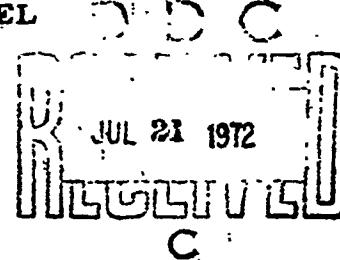


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A HIGH ALTITUDE RADIANCE MODEL

Thomas C. Degges

Visidyne, Inc.
169 Merrimac Street,
Woburn, Massachusetts 01801



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13. ABSTRACT A knowledge of the natural infrared radiance originating in the earth's upper atmosphere is of interest for systems design, military surveillance and the advancement of knowledge about physical processes in the upper atmosphere. A physical model that includes experimental data on and theoretical estimates of excitation processes that lead to emission of infrared radiation has been implemented in a computer program that computes infrared radiances for an earth's limb viewing geometry. The nominal spectral region of this study lies between five and twenty-five micrometers and emphasis is placed on radiation originating at altitudes between 70 and 500 km. An earlier model for the transport of infrared radiation in molecular bands with Doppler line shape, accurate only for linear molecules, has been extended to bands of polyatomic molecules. A chemistry program which includes the effects of vertical transport by eddy mixing and molecular diffusion has been developed to make possible an estimate of diurnal variation in the abundances of infrared emitting species. Computational results are given for the latitude of

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SECTION I

INTRODUCTION

The research reported here has had as its major objective the development of a computer program to simulate the natural infrared radiance background of the earth's upper atmosphere. The nominal spectral region under study lies between five and twenty-five micrometers and emphasis is placed on radiation originating at altitudes between 70 and 500 kilometers. The general problem area is of interest for systems design, military surveillance and the advancement of knowledge about physical processes in the upper atmosphere. The immediate application of this work will be to aid in developing optimum infrared background measurements programs and in interpreting the results of such measurements.

This work is an extension of the study of Corbin, et al. (1969) who investigated the natural infrared background of the earth in the 5 to 25 micrometer spectral region, with the goal of estimating earth limb viewing radiances for tangent heights from the surface to 500 km altitude. For convenience, their study divided the atmosphere into two regions with a division at 70 km. Below 70 km the atmosphere was assumed to be in thermal equilibrium. Above 70 km explicit calculations were made of processes which excite and de-excite molecular vibrational and rotational levels which are the source of infrared radiation. Their study concentrated on radiation from water vapor, carbon dioxide, ozone, nitric oxide and nitrous oxide, which are the principal radiating

species in the spectral region considered. In addition, nitric acid was included in the lower atmosphere work and estimates were made of radiation to be expected from particulate matter suspended in the atmosphere.

Corbin, et al. (1969) presented models for the lower atmosphere for a wide range of seasonal and latitudinal conditions. This was not possible for the abundances of most minor neutral species. More data has since become available, particularly for nitric oxide and the hydroxyl radical, but at present it appears that the best means of estimating abundances of important infrared emitting species is chemical rate equation integrations including molecular diffusion and eddy mixing. Even calculations involving transport properties cannot always be accepted because the values of eddy mixing coefficients are to a large extent only informed guesses and published calculations often use outdated rate coefficients. For these reasons, one of the tasks of the current contract has been to develop a computer program with which to determine diurnal variations in abundances of minor species, to investigate the effects of changes in assumed eddy mixing coefficients, and to quickly incorporate new determinations of chemical rate coefficients.

A second area of study involved in improving the radiance model includes the physical processes that control the population of infrared emitting states of atmospheric molecules. Except for the pure rotational radiation from molecules such as water, the degree of excitation of vibrational levels determines the radiation from infrared emitting molecules. The most important mechanisms are collisional excitation and de-excitation and absorption and re-emission of electromagnetic radiation.

In the troposphere and lower stratosphere, collisional processes are rapid enough to control the population of vibrational levels. Above 30 to 50 km, however, collisional excitation becomes less efficient and radiative processes become important. The combined effects of collisional and radiative processes must therefore be considered. Below an altitude of about 90 km molecular nitrogen and oxygen are the most important collision partners. Above that

altitude, atomic oxygen becomes important, both in exciting nitric oxide and in determining molecular oxygen vibrational temperatures. Corbin, et al. (1969) included collisional excitation by molecular nitrogen and oxygen in their model and the work reported here adds the effects of atomic oxygen as a collision partner.

In determining the effects of radiation on the populations of vibrational levels of infrared active molecules, it is necessary to separate the radiation of a single change in vibrational quantum numbers from the rest of the radiation field. Corbin et al. (1969) did this by assuming a Doppler line shape for the individual rotational lines of a band and were able to obtain adequate numerical approximations for radiative transfer functions appropriate to single bands of linear molecules. This approach has been extended to water vapor and ozone bands lying in the spectral region of interest.

The following sections of this report summarize the research performed during this contract. The computational algorithm used in the chemistry program, relevant chemical reaction rate coefficients and currently known chemical abundances in the upper atmosphere are discussed in Section II. Relevant collisional and radiative excitation mechanisms are reviewed in Section III, where the computational model for predicting high altitude infrared radiance is developed. The chemistry and infrared radiance programs are described and listed in Section IV. Sample results for White Sands, New Mexico are presented in Section V, where limitations of the model and suggestions for future work are discussed.

SECTION II

CHEMISTRY

There have been relatively few measurements of the variation with altitude of infrared emitting species at altitudes above 30 km, the limit of direct sampling by balloons. While ozone measurements by different workers agree reasonably well with each other and with theoretical computations at altitudes up to 100 km, and nitric oxide profiles are reasonably well known between about 80 and 150 km, corresponding data are lacking for other species which are important. There is in some cases indirect data available which when combined with computational models can yield limits to concentrations. Thus, Anderson (1971a) has been able to put an upper limit on total hydroxyl radical abundance above 60 km from measurement of resonance fluorescence and with this result computes possible water vapor profiles between 50 and 100 km using a photochemical model that includes vertical transport by eddy diffusion. In a later paper, Anderson (1971b) gives a measured altitude profile for hydroxyl with error limits ± 120 per cent.

At present, then, estimates of chemical abundances of minor species required to predict infrared radiation require the use of photochemical computations. Most computations of atmospheric chemistry before the past four or five years have neglected vertical transport by molecular diffusion and eddy mixing. For molecules which have photochemical lifetimes greater than 10^4 to 10^5 seconds, this neglect may yield results greatly in error, as a comparison of the calculations of Hunt (1966), Hesstvedt (1968) and Shimazaki

and Laird (1970) quickly shows. Even calculations including transport processes cannot be accepted at face value because the values of eddy mixing coefficients used at present are for the most part only informed estimates, and published calculations often use outdated rate coefficients. Because of the above reasons, and the future need to estimate abundances for conditions for which no published experimental data or calculations may be available, development of a computational model for atmospheric photochemistry including vertical transport was considered desirable. The present status of this model is described below.

Following Shimazaki and Laird (1970) and Bowman, et al. (1970), the continuity equation for an atmospheric chemical constituent or species may be written

$$\frac{\partial n(z)}{\partial t} = Q(z) - L(z) - \frac{\partial \Phi(z)}{\partial z} \quad (2-1)$$

where n is the concentration of the constituent, Q and L are photochemical production and loss rates and Φ is the vertical flux due to transport processes. When only vertical transport by molecular diffusion and eddy or turbulent mixing is considered, the vertical flux is

$$\Phi(z) = n(z)u(z) + n(z)v(z) \quad (2-2)$$

where u and v are vertical velocities of the species produced by molecular diffusion and eddy mixing, respectively. If D is an "average" molecular diffusion coefficient, H is the scale height of the species in the absence of

mixing and T is the temperature,

$$u(z) = -D \left(\frac{\partial n}{\partial z} + \frac{n}{H} + \frac{n}{T} \frac{\partial T}{\partial z} \right) \quad (2-3)$$

If K is the eddy mixing coefficient and H_{av} is the average scale height for all species present,

$$v(z) = -K \left(\frac{\partial n}{\partial z} + \frac{n}{H_{av}} + \frac{n}{T} \frac{\partial T}{\partial z} \right) \quad (2-4)$$

Then

$$\frac{\partial n(z)}{\partial t} = Q(z) - L(z) + \frac{\partial}{\partial z} \left[(D+K) \left(\frac{\partial n}{\partial z} + \frac{n}{T} \frac{\partial T}{\partial z} \right) + \left(\frac{D}{H} + \frac{K}{H_{av}} \right) n \right] \quad (2-5)$$

As was done by Bowman, et al. (1970), it is assumed that only atomic oxygen and molecular nitrogen and oxygen are important as collision partners. The effective diffusion coefficients for atomic oxygen and molecular nitrogen and oxygen are taken to be

$$D_i(z) = N_o \left(\frac{T(z)}{T_o} \right)^{0.75} \left/ \sum_{j=1}^3 \frac{n_j(z)}{D_{ij}} \right. \quad (2-6)$$

where N_o is number density at standard temperature and pressure (STP), T_o is 273.15 K, and the D_{ij} are mutual diffusion coefficients at STP. The

values adopted for $D_{O_2-N_2}$, D_{O-O_2} and D_{O-N_2} are those used by Colegrove, et al. (1966), 0.181, 0.260 and 0.260, respectively. That for $D_{O_2-O_2}$, 0.189, is taken from Chapman and Cowling (1960), while $D_{N_2-N_2}$ and D_{O-O} are estimated to be 0.180 and 0.370. The effective diffusion coefficients for other species are taken to be

$$D_i = 0.707 D_{O_2} \left(1 + \frac{m(O_2)}{m_i} \right)^{1/2} \quad (2-7)$$

where m_i represents molecular weight.

In converting Equation (2-5) into a difference scheme for numerical integration, it is assumed that all quantities may be represented by a quadratic function of altitude at any given altitude. Then if the superscript (+) denotes a value at the next higher integration point and the superscript (-) denotes a value at the next lower point, the difference equation is

$$\begin{aligned} \frac{\partial n}{\partial t} = & Q - L + \frac{D^+ - D^-}{2\Delta z} \left[\frac{n^+ - n^-}{2\Delta z} + \left(\frac{1}{T} \frac{T^+ - T^-}{2\Delta z} + \frac{1}{H} \right) n \right] \\ & + \frac{K^+ - K^-}{2\Delta z} \left[\frac{n^+ - n^-}{2\Delta z} + \left(\frac{1}{T} \frac{T^+ - T^-}{2\Delta z} + \frac{1}{H_{av}} \right) n \right] \\ & + (D + K) \left[\frac{n^+ - 2n + n^-}{(\Delta z)^2} - \left(\frac{1}{T} \frac{T^+ - T^-}{2\Delta z} \right)^2 n + \frac{1}{T} \left(\frac{T^+ - 2T + T^-}{(\Delta z)^2} \right) n \right. \\ & \left. + \frac{1}{T} \left(\frac{T^+ - T^-}{2\Delta z} \right) \left(\frac{n^+ - n^-}{2\Delta z} \right) + \frac{1}{H} \left(\frac{n^+ - n^-}{2\Delta z} \right) - \frac{n}{H^2} \left(\frac{H^+ - H^-}{2\Delta z} \right) \right] \\ & + D \left[\frac{1}{H} \left(\frac{n^+ - n^-}{2\Delta z} \right) - \frac{n}{H^2} \left(\frac{H^+ - H^-}{2\Delta z} \right) \right] + K \left[\frac{1}{H_{av}} \left(\frac{n^+ - n^-}{2\Delta z} \right) - \frac{n}{H_{av}^2} \left(\frac{H_{av}^+ - H_{av}^-}{2\Delta z} \right) \right] \end{aligned} \quad (2-8)$$

The computational problem then is simply to integrate Equation (2-8) at a set of altitudes with spacing Δz , taking successive time steps $h = \Delta t$ over the desired time of interest. The method used takes advantage of the observation that except where a species is important as a third body in an association reaction which removes it, the chemical rate equations for a coupled system may be cast in the form

$$x_i' = q_i(x) - \beta_i(x)x_i - \alpha_i(x)x_i^2 \quad (2-9)$$

with formal solutions (assuming q , α and β constant and omitting obvious subscripts)

$$x_i(t) = \frac{[(\beta + \delta) \exp(-\delta t) + (\delta - \beta)]x_i(0) + 2q[1 - \exp(-\delta t)]}{(2\alpha x_i(0) + \beta)[1 - \exp(-\delta t)] + [1 + \exp(-\delta t)]\delta}$$

$$q > 0, \beta > 0, \alpha > 0 \quad (2-10a)$$

where

$$\delta = (4\alpha q + \beta^2)^{1/2}$$

$$x_i(t) = x_i(0) \exp(-\beta t) + q[1 - \exp(-\beta t)]/\rho$$

$$q > 0, \beta > 0, \alpha = 0 \quad (2-10b)$$

$$x_i(t) = \frac{[1 + \exp(-\delta t)]x_i(0)\delta + 2q[1 - \exp(-\delta t)]}{2\alpha x_i(0)[1 - \exp(-\delta t)] + [1 + \exp(-\delta t)]\delta}$$

$$q > 0, \beta = 0, \alpha > 0 \quad (2-10c)$$

where

$$\delta = (4\alpha q)^{1/2}$$

$$x_i(t) = x_i(0) + qt \quad q > 0, \beta = 0, \alpha = 0 \quad (2-10d)$$

$$x_i(t) = \frac{\beta x_i(0) \exp(-\beta t)}{\alpha x_i(0)[1 - \exp(-\beta t)] + \beta}, \quad q = 0, \beta > 0, \alpha > 0 \quad (2-10e)$$

$$x_i(t) = x_i(0) \exp(-\beta t), \quad q = 0, \beta > 0, \alpha = 0 \quad (2-10f)$$

$$x_i(t) = x_i(0)/[1 + \alpha t x_i(0)] \quad q = 0, \beta = 0, \alpha > 0 \quad (2-10g)$$

$$x_i(t) = x_i(0), \quad q = 0, \beta = 0, \alpha = 0 \quad (2-10h)$$

Care must be exercised in the definition of the α and β terms. For example, the reaction



contributes to both the α and the β terms in the differential equation for O_2^+ concentration if other positive ions are present;

$$\alpha = k$$

$$\beta = k([e] - [O_2^+])$$

The solutions, Equation (2-10), are exact only if q , β , and α do not change during an integration interval. Since q , β , and α are functions of the time dependent concentrations of the other species in the system, the actual integration scheme must allow for this variation.

If the time step $t \ll 2/|2\alpha x + \beta - \delta|$ and $\delta t \ll 2$, the denominator of Equation (2-10a) may be expanded as $1 - (2\alpha x + \beta - \delta)t/2\delta$ and

$$x_i(t) = x_i(0) + (q_i - \beta_i \dot{x}_i(0) - \alpha_i x_i^2(0))t + O(t^2). \quad (2-11)$$

For a small enough time step, the algorithm is equivalent to Euler's method. With the same restrictions on the time step, the algorithm may be embedded in

a Runge-Kutta formula of any order and will give equivalent results.

The program uses an analog of the improved tangent second-order Runge-Kutta method in the basic step h . Let $x(0)$ be the value of a dependent variable at the beginning of the step. Then $\alpha(0)$, $\beta(0)$ and $q(0)$ are computed and a new value of x computed for $t = \frac{1}{2}h$ from the general expression, Equation (2-10a), or from an equivalent expression, if any α , β or q is equal to zero. $\alpha(h/2)$, $\beta(h/2)$ and $q(h/2)$ are computed and Equation (2-10) evaluated with these values and $t = h$.

Following Ceschino and Kuntzmann (1966), assume that the stepsize is chosen so that a linearized theory of errors may be applied. That is, for a method of order n , the error for one step of length h is Ah^{n+1} . Divide an interval Ht into an even number k of steps of length h . Then

$$x_i^{(h)}(t) = x_i^{(0)}(t) + kAh^{n+1} + O(h^{n+2}) \quad (2-12)$$

where $x_i^{(0)}(t)$ is the "exact" result of the integration and addition or subtraction of the error by propagation is neglected. The result using a step of length $2h$ is

$$x_i^{(2h)}(t) = x_i^{(0)}(t) + k/2 A(2h)^{n+1} + O(h^{n+2}) \quad (2-13)$$

The difference between the two results is

$$x_i^{(2h)}(t) - x_i^{(h)}(t) \approx kAh^{n+1}(2^n - 1) \quad (2-14)$$

and the principal part of the error using the step h is

$$\epsilon_h \approx \frac{x_i^{(2h)}(t) - x_i^{(h)}(t)}{2^n - 1} \quad (2-15)$$

The simplest way to use this result is to divide an interval into two equal steps h and integrate twice, once with two steps of length h and then with one step of length $2h$. The principal part of the error may be used both to correct the result $x_i^{(2h)}(t)$ and to estimate the optimum length of the next interval of integration. The Runge-Kutta integration program of Gear (1971) is easy to adapt for both uses of the error estimate, and was used in early tests.

It is more efficient to use Romberg extrapolation, which subdivides an interval H in more than two ways, and uses higher order error terms. Either polynomial Romberg extrapolation [Davis and Rabinowitz, (1967)] or rational Romberg extrapolation [Bulirsch and Stoer (1966)] may be used.

Denote the result of integrating from the $t = 0$ to $t = H$ with a constant step size h by $X(h)$. Assume that $X(h)$ has an asymptotic expansion

$$X(h) = \xi_0 + \xi_1 h^{\gamma_1} + \xi_2 h^{\gamma_2} + \dots \quad (2-16)$$

with $\xi_0, \xi_1, \xi_2, \dots$ constant, so that in the limit $h \rightarrow 0$, $X(0) = \xi_0$.

the exact solution. An approximation to $X(0)$ may be obtained by extrapolation from the results of integration with finite values of h .

Let the global interval of integration H be successively divided into 2, 3, 4, 6, 8, 12, ... intervals with $h = \frac{1}{2}H, \frac{1}{3}H, \frac{1}{4}H, \frac{1}{6}H, \dots$

Let $X_0^{(0)}(H)$ be the value obtained with $h = \frac{1}{2}H$, $X_0^{(1)}(H)$ be that obtained from $h = \frac{1}{3}H$, etc. Then a table of extrapolated values

$$\begin{array}{ccccccc}
 & & X_0^{(0)}(H) & & & & \\
 & X_0^{(1)}(H) & & X_1^{(0)}(H) & & & \\
 & X_0^{(2)}(H) & & X_1^{(1)}(H) & & X_2^{(0)}(H) & \\
 & X_0^{(3)}(H) & & X_1^{(2)}(H) & & X_2^{(1)}(H) & & X_3^{(0)}(H) & (2-17) \\
 & \dots & & \dots & & \dots & & \dots & \\
 & X_0^{(m)}(H) & & X_1^{(m-1)}(H) & & X_2^{(m-2)}(H) & & X_3^{(m-3)}(H) & \dots X_m^{(0)}(H)
 \end{array}$$

is computed using

$$X_1^{(0)}(H) = \frac{A_1^{(0)} X_0^{(1)}(H) - X_0^{(0)}(H)}{A_1^{(0)} - 1}$$

$$x_1^{(1)}(H) = \frac{A_1^{(1)} x_0^{(2)}(H) - x_0^{(1)}(H)}{A_1^{(1)} - 1} \quad x_2^{(0)}(H) = \frac{A_2^{(0)} x_1^{(1)}(H) - x_1^{(0)}(H)}{A_2^{(0)} - 1}$$

.....

(2-18)

$$x_k^{(j)}(H) = \frac{A_k^{(j)} x_{k-1}^{(j+1)}(H) - x_{k-1}^{(j)}(H)}{A_k^{(j)} - 1}$$

If the method used in integrating over a step h is of order n , the exponents in Equation (2-16) have the values

$$\gamma_i = n - 1 + i \quad (2-19)$$

Equation (2-16) may be written out for as many values of h as desired and these equations solved simultaneously. The coefficients $A_k^{(j)}$ of Equation (2-18) are obtained from the multipliers used in solving such a system of algebraic equations. Table II-1 gives the coefficients $A_k^{(j)}$ for $k = 1, 2, \dots, 9$ for first, second, third and fourth order integration methods. Only the second order coefficients are used here.

Subdivision of the basic interval is continued until the value of

Table II-1

Coefficients $A_k^{(j)}$ for Polynomial Extrapolation

using Subintervals $H/2, H/3, H/4, H/6, H/8, \dots$

k	First Order		Second Order		Third Order		Fourth Order	
	j even	j odd	j even	j odd	j even	j odd	i even	j odd
1	$\frac{3}{2}$	$\frac{4}{3}$	$\frac{9}{4}$	$\frac{16}{9}$	$\frac{27}{8}$	$\frac{64}{27}$	$\frac{81}{16}$	$\frac{256}{81}$
2	2	2	$\frac{20}{7}$	$\frac{14}{5}$	$\frac{152}{37}$	$\frac{74}{19}$	$\frac{208}{35}$	$\frac{70}{13}$
3	3	$\frac{8}{3}$	$\frac{13}{3}$	$\frac{48}{13}$	$\frac{69}{11}$	$\frac{352}{69}$	$\frac{173}{19}$	$\frac{1216}{173}$
4	4	4	$\frac{40}{7}$	$\frac{28}{5}$	$\frac{2320}{283}$	$\frac{1132}{145}$	$\frac{1760}{149}$	$\frac{596}{55}$
5	6	$\frac{16}{3}$	$\frac{198}{23}$	$\frac{736}{99}$	$\frac{582}{47}$	$\frac{3008}{291}$	$\frac{9666}{541}$	$\frac{69248}{4833}$
6	8	8	$\frac{80}{7}$	$\frac{56}{5}$	$\frac{3424}{209}$	$\frac{1672}{107}$	$\frac{23360}{991}$	$\frac{7928}{365}$
7	12	$\frac{32}{3}$	$\frac{292}{17}$	$\frac{1088}{73}$	$\frac{7716}{313}$	$\frac{40064}{1929}$	$\frac{89476}{2521}$	$\frac{645376}{22369}$
8	16	16	$\frac{160}{7}$	$\frac{112}{5}$	$\frac{43072}{1315}$	$\frac{21040}{673}$	$\frac{10880}{231}$	$\frac{3696}{85}$
9	24	$\frac{64}{3}$	$\frac{3672}{107}$	$\frac{13696}{459}$	$\frac{3592}{73}$	$\frac{18688}{449}$	$\frac{11112}{157}$	$\frac{80384}{1389}$

$$\left(x_k^{(o)} - x_{k-1}^{(o)} \right) / x_k^{(o)}$$

is less than a preassigned value ϵ . In practice, adequate results are obtained if for $k > 6$ the test is on values of

$$\left(x_6^{(j)} - x_6^{(j-1)} \right) / x_6^{(j)} .$$

The chief advantage of this integration method is that large time intervals may be used and the algorithm contains an error estimate.

As applied in the program, the L term in Equation (2-8) is divided into two parts, αn^2 and βn . To the Q term is added the terms containing n^+ and n^- . The multipliers of the terms in n are added to the β term from the photochemistry and Equation (2-10) is used with interval subdivision and polynomial Romberg extrapolation as described above.

Table II-2 lists the main neutral reactions which may play a role in the chemistry of the infrared emitting molecules NO , CO_2 , H_2O , O_3 , N_2O and CH_4 . Table II-3 lists the photodissociation processes considered. Table II-4 lists the ionic reactions needed for nitric oxide chemistry. Where possible, an estimated error is given for the value of the rate coefficient. Critical reviews are the principal source of rates listed here and in most cases newer rates from the literature fall within estimated error limits.

Not all the reactions listed in Table II-2 have been included in the program, as some occur in branching chains which have not been verified in

Table II-2

Reaction Rates for Neutral Species

Reactants and products are in lowest electronic state unless indicated explicitly.
Where two rates are given, (a) is for the reaction as written, (b) is for the reverse.

<u>Reaction</u>	<u>Rate Coefficient, c. g. s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R1a $O + O + M \rightarrow O_2 + M$	$3.8 \times 10^{-30} T^{-1} \exp(-171/T)$	Johnston (1968)	High by up to 50%
R1b	$4.57 \times 10^{-5} T^{-1} \exp(-59700/T)$	Johnston (1968)	30%
R2a $O + O_2 + M \rightarrow O_3 + M$	$4.63 \times 10^{-35} \exp(1060/T)$	Johnston (1968)	30%
R2b	$1.65 \times 10^{-9} \exp(-11420/T)$	Johnston (1968)	30%
R3a $O + O_3 \rightarrow 2O_2$	$2.0 \times 10^{-11} \exp(-2410/T)$	Johnston (1968)	30%
R3b	$2.12 \times 10^{-11} \exp(-50700/T)$	Johnston (1968)	30%
R4 $H + O_3 \rightarrow OH + O_2$	2.6×10^{-11}	Kaufman (1969)	20% at 300 K
R5a $O + OH \rightarrow H + O_2$	2.06×10^{-11}	Schofield (1967)	50%
R5b	$4.19 \times 10^{-10} \exp(-8450/T)$	Schofield (1967)	50%
R6 $O + HO_2 \rightarrow OH + O_2$	$\geq 10^{-11}$	Kaufman (1969)	
R7 $H + HO_2 \rightarrow H_2O + O$	$2.0 \times 10^{-10} \exp(-2000/T)$	Bates and Niccolot (1950)	An estimate
R8 $H + O_2 + M \rightarrow HO_2 + M$	$3.0 \times 10^{-32} (273/T)^{1.3}$	Schofield (1967)	30%

<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R9 $\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	5.0×10^{-13}	Kaufman (1969)	
R10 $\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2\text{O}_2$	10^{-14}	Hunt (1964)	An estimate
R11a $\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	$9.3 \times 10^{-12} \exp(-390/T)$	Baulch, et al. (1968b)	20% at 300 K
R11b $\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$	$9.3 \times 10^{-11} \exp(-9000/T)$	Baulch, et al. (1968b)	20% at 300 K
R12 $\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$	$\gg 10^{-11}$	Kaufman (1969)	See Text
R13 $\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	2.0×10^{-13}	Clyne and Thrush (1963)	30%
R14 $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$	$7.0 \times 10^{-11} \exp(-5100/T)$	Wong and Potter (1965)	30%
R15 $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1.5×10^{-12}	Kaufman (1969)	30%
R16 $\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{HO}_2$	4.0×10^{-13}	Foner and Hudson (1962)	50%
R17 $\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{HO}_2$	10^{-15}	Foner and Hudson (1962)	50%
R18 $\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	10^{-13}	Foner and Hudson (1962)	50%
R19a $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$* 3.6 \times 10^{-11} \exp(-2600/T)$	Baulch, et al. (1968b)	35% at 300 K
R19b $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$* 1.4 \times 10^{-10} \exp(-10^4 T)$	Baulch, et al. (1968b)	35% at 300 K
R20 $\text{O} + \text{H} + \text{M} \rightarrow \text{OH} + \text{M}$	$* 8.0 \times 10^{-33}$	Bates and Nicolet (1950)	Estimate
R21 $\text{O} + \text{OH} + \text{M} \rightarrow \text{HO}_2 + \text{M}$	$* 1.4 \times 10^{-31}$	Kaufman (1964)	30%

	<u>Reaction</u>	<u>Rate Coefficient, c. g. s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R22	$H + H + M \rightarrow H_2 + M$	$* 1.2 \times 10^{-32} (273/T)^0.7$	Kaufman (1969)	30%
R23	$H + OH + M \rightarrow H_2O + M$	$* 2.5 \times 10^{-31}$	Kaufman (1964)	50%
R24	$H + HO_2 \rightarrow 2OH$	$* \geq 3 \times 10^{-12}$	Kaufman (1969)	
R25	$H + HO_2 \rightarrow H_2 + O_2$	$* \geq 3 \times 10^{-12}$	Kaufman (1969)	
R26	$H + OH \rightarrow H_2 + O$	$* 3.0 \times 10^{-11} \exp(-4170/T)$	Kaufman (1969)	30%
R27	$O(^1D) + N_2 \rightarrow O(^3P) + N_2$	5.0×10^{-11}	Donovan and Husain (1970)	50%
R28	$O(^1D) + O_3 \rightarrow O_2 + O_2$	5.0×10^{-11}	Snelling and Bair (1969)	50%
R29	$O(^1D) + H_2 \rightarrow OH + H$	1.0×10^{-11}	Donovan and Husain (1970)	Uncertain
R30	$O(^1D) + H_2O \rightarrow OH + OH$	3.0×10^{-11}	Donovan and Husain (1970)	Uncertain
R31	$O(^1D) + H_2O \rightarrow OH + OH$	$* 10^{-11}$	Estimate	
R32	$O(^1D) + CH_4 \rightarrow Products$	10^{-11}	Donovan and Husain (1970)	Uncertain
R33	$CO + OH \rightarrow CO_2 + H$	$1.0 \times 10^{-12} \exp(-540/T)$	Baulch, et al. (1968a)	30%
R34	$CO + O + M \rightarrow CO_2 + M$	$1.4 \times 10^{-33} \exp(-1250/T)$	Baulch, et al. (1968a)	Extremely uncertain
R35	$CO + HO_2 \rightarrow CO_2 + OH$	$* 2.5 \times 10^{-17}$	Schofield (1967)	Uncertain
R36	$CH_4 + OH \rightarrow H_2O + CH_3$	$1.2 \times 10^{-10} \exp(-2960/T)$	Schofield (1967)	30%
R37	$O + CH_4 \rightarrow OH + CH_3$	$3.5 \times 10^{-11} \exp(-4550/T)$	Herron (1969)	50%

<u>Reaction</u>	<u>Rate Coefficient, c. g. s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R.38 $\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$	$*5.0 \times 10^{-11} \exp(-5000/T)$	Dean and Kistiakowski (1971)	Uncertain
R.39 $\text{CH}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCO}$	$*5.3 \times 10^{-10} \exp(-2120/T)$	Schofield (1967)	50%
R.40 $\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{HCO}$	$*7.5 \times 10^{-15}$	Schofield (1967)	Uncertain
R.41 $\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	$*1.0 \times 10^{-13}$	Estimate	Uncertain
R.42a $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$	$1.1 \times 10^{-14} T \exp(-3140/T)$	Baulch, et al. (1969)	30% at 300 K
R.42b	$2.6 \times 10^{-15} T \exp(-19500/T)$	Baulch, et al. (1969)	30%
R.43a $\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$	$5.1 \times 10^{-11} \exp(-168/T)$	Baulch, et al. (1969)	Factor of 2
R.43b	$2.3 \times 10^{-10} \exp(-37500/T)$	Baulch, et al. (1969)	Factor of 2
R.44a $\text{NO} + \text{NO} \rightarrow \text{N}_2 + \text{O}_2$	$1.3 T^{-5/2} \exp(-42800/T)$	Freedman and Daiber (1961)	Highly uncertain
R.44b	$15.2 T^{-5/2} \exp(-64300/T)$	Wray and Teare (1962)	Highly uncertain
R.45 $\text{N} + \text{N} + \text{M} \rightarrow \text{N}_2 + \text{M}$	$1.4 \times 10^{-33} \exp(-500/T)$	Schiff (1969)	Factor of 2
R.46a $\text{N} + \text{O} + \text{M} \rightarrow \text{NO} + \text{M}$	$1.1 \times 10^{-32} (273/T)^{1/2}$	Baulch, et al. (1969)	50%
R.46b	$3.8 \times 10^{-7} T^{-1/2} \exp(-74500/T)$	Baulch, et al. (1969)	Factor of 5
R.47 $\text{O} + \text{NO} \rightarrow \text{NO}_2 + \text{h}\nu$	$6.5 \times 10^{-17} (T/296)$	Baulch, et al. (1970)	Factor of 2
R.48 $\text{O} + \text{NO}_2 \rightarrow \text{NO} + \text{O}_2$	$1.6 \times 10^{-11} \exp(-300/T)$	Baulch, et al. (1970)	20%

<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R49 N + NO ₂ → N ₂ O + O	*7.8 x 10 ⁻¹²	Schiff (1969)	30% at 300 K
R50 N + NO ₂ → N ₂ + 2O	2.3 x 10 ⁻¹²	Schiff (1969)	Factor of 2 at 300 K
R51 N + NO ₂ → N ₂ + O ₂	*1.8 x 10 ⁻¹²	Schiff (1969)	Factor of 2 at 300 K
R52 N + NO ₂ → 2NO	5.9 x 10 ⁻¹²	Schiff (1969)	30% at 300K
R53a NO + O + M → NO ₂ + M	2.9 x 10 ⁻³³ exp(940/T)	Baulch,etal.(1970)	20%
R53b	1.8 x 10 ⁻⁸ exp(-32800/T)	Baulch,etal.(1970)	25% at 1500 K
R54a NO + NO + O ₂ → NO ₂ + NO ₂	6.6 x 10 ⁻³⁹ exp(530/T)	Baulch,etal.(1970)	50%
R54b	6.6 x 10 ⁻¹² exp(-13500/T)	Baulch,etal.(1970)	50%
R55 O ₃ + NO → NO ₂ + O ₂	9.5 x 10 ⁻¹³ exp(-1240/T)	Schiff (1969)	30%
R56 N + O ₂ (Δ _g ¹) → NO + O	*3.0 x 10 ⁻¹⁵	Clark and Wayne (1969)	30%
R57 N + O ₃ → NO + O ₂	*3.0 x 10 ⁻¹¹ exp(-1200/T)	Nicollet (1965)	An estimate
R58 N(² D) + O ₂ → NO + O	6.0 x 10 ⁻¹²	Lin and Kaufman (1969)	20% at 300 K
R59 N(² D) + N ₂ O → NO + N ₂	*3.6 x 10 ⁻¹³ T ^{1/2} exp(-400/T)	Sanger,etal.(1971)	50%
R60 N + OH → NO + H	*6.8 x 10 ⁻¹¹	Campbell and Thrush (1968)	20% at 320 K
R61 N(² D) + O → N(⁴ S) + O	2.0 x 10 ⁻¹³	Weill (1969)	An estimate

*An asterisk preceding the rate coefficient indicates that the reaction is not included in the present version of the chemistry program.

Table II-3

Photodissociation Processes Considered for Chemistry Program

	Reaction	Source of Cross Sections
J1	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	Hudson, Carter and Breig (1969) Ackerman (1970)
J2	$O_2 + h\nu \rightarrow O(^1D) + O(^3P)$	Ackerman (1970)
J3	$O_3 + h\nu \rightarrow O(^3P) + O_2$	Ackerman (1970)
J4	$O_3 + h\nu \rightarrow O(^1D) + O_2$	Ackerman (1970)
J5	$H_2O + h\nu \rightarrow OH + H$	Watanabe, et al. (1953)
J6	$H_2O_2 + h\nu \rightarrow OH + OH$	Schurnb, et al. (1955)
J7	$HC_2 + h\nu \rightarrow OH + O(^3P)$	Assumed same as H_2O_2
J8	$NO + h\nu \rightarrow NO^+ + e^-$	Donahue (1966)
J9	$NO_2 + h\nu \rightarrow NO + O(^3P)$	Hall and Blacet (1952)
J10	$NO_2 + h\nu \rightarrow N(^4S) + O_2$	Strobel (1971b)
J11	$N_2O + h\nu \rightarrow NO + N(^4S)$	Zelikoff, et al. (1953)
J12	$N_2 + h\nu \rightarrow 2N(^4S)$	Hudson and Carter (1969)
J13	$CO_2 + h\nu \rightarrow CO + O$	Watanabe, et al. (1953)
J14	$CH_4 + h\nu \rightarrow CH_3 + \cdot$	Watanabe, et al. (1953)

Solar fluxes for Lyman- α (1216 Å) and wavelengths longer than 1170 Å were taken from Ackerman (1970). Selection of cross section data was aided by the review of Hudson (1971).

Table II-4

Ionic Reactions Required for Nitric Oxide Chemistry

	<u>Reaction</u>	<u>Rate Coefficient, cgs units</u>	<u>Source</u>
IIa	$N^+ + C_2 \rightarrow NO^+ + O$	6.0×10^{-10}	Fehsenfeld, et al. (1969)
IIb	$N^+ + O_2 \rightarrow O_2^+ + N$		
IIc	$O^+ + N_2 \rightarrow NO^+ + N$	6.0×10^{-13} (600/T)	Dunkin, et al. (1968)
II-12	$O^+ + O_2 \rightarrow O_2^+ + O$	$1.1 \times 10^{-9} T^{-0.7}$	Dunkin, et al. (1968)
II-13	$O^+ + O_2 \rightarrow O_2^+ + O$	2.0×10^{-11}	Goldan, et al. (1966)
II-14	$O^+ + NO \rightarrow NO^+ + O$	1.0×10^{-9}	Dalgarno and McElroy (1966)
II-15	$O^+ ({}^2D) + N_2 \rightarrow N_2^+ + O$	1.0×10^{-7}	Hunten and McElroy (1966)
II-16	$O^+ ({}^2D) + e \rightarrow O^+ ({}^4S) + e$	1.4×10^{-10}	Fehsenfeld, et al. (1970)
II-17a	$N_2^+ + O \rightarrow NO^+ + N({}^4S)$	2.8×10^{-7}	Kasner and Biondi (1965)
II-17b	$N_2^+ + O \rightarrow NO^+ + N({}^2D)$	$6.0 \times 10^{-11} (300/T)^{0.6}$	Johnson, et al. (1970)
II-18a	$N_2^+ + e \rightarrow 2N({}^4S)$	3.3×10^{-10}	Fehsenfeld, et al. (1970)
II-18b	$N_2^+ + e \rightarrow N({}^2D) + N({}^4S)$	1.8×10^{-10}	Goldan, et al. (1966)
II-19	$N_2^+ + O_2 \rightarrow O_2^+ + N_2$	6.3×10^{-10}	Fehsenfeld, et al. (1970)
II-10	$N_2^+ + NO \rightarrow NO^+ + N_2$	$6.6 \times 10^{-5}/T$	Bjordi (1969)
II-11	$O_2^+ + N \rightarrow NO^+ + O$	$1.0 \times 10^{-7} (T/1000)^{-1.5}$	Weller and Biondi (1968)
II-12	$O_2^+ + NO \rightarrow NO^+ + O_2$	$< 2 \times 10^{-16}$	Shahin (1967)
II-13	$O_2^+ + e \rightarrow 2O$		
II-14a	$NO^+ + e \rightarrow N({}^4S) + O$		
II-14b	$NO^+ + e \rightarrow N({}^2D) + O$		
II-15	$O_2^+ + N_2 \rightarrow NO^+ + NO$		

the laboratory. The choice of reactions has been guided by those used in published calculations and reviews. The most uncertain rates are those involving the carbon compounds. These have been studied principally at elevated temperatures and extrapolation to the low temperatures of the upper stratosphere and mesosphere is not reliable.

The results of Nicolet (1970) and Bowman, et al. (1971) were used as a guide to the selection of reactions to include in the chemistry of oxygen and hydrogen compounds. Rates for Reactions R1, R2 and R3 were taken from Johnston (1968) in preference to other sources because they are thermodynamically consistent for the $O-O_2-O_3$ system. The rates for nitric oxide reactions follow closely those used by Stroebel (1971a, 1971b). The choice of reactions for methane decomposition is based on the partial kinetic systems of Herron (1969) and Hoare and Patel (1969). Reactions leading to formation of CH_2 have been omitted.

Of the chemical species considered here, nitric oxide abundances are best known above an altitude of 70 km. Observations of solar ultraviolet induced fluorescence in the gamma bands have been made by Barth (1964, 1966a, 1966b), Pearce (1969a) and Meira (1971). Abundances measured in this way are much higher than predicted by earlier photochemical theories such as those of Nicolet (1965a, 1965b). Norton and Barth (1970) and Stroebel, et al. (1970) showed that $N(^2D)$ produced in dissociative recombination of NO^+ (Reaction II4b) and in charge exchange of N_2^+ with atomic oxygen (Reaction I7b) could form sufficient nitric oxide in reacting with molecular oxygen to explain measured abundances. The amount of $N(^2D)$ formed in the relevant reactions has not been determined in the laboratory and remains an adjustable parameter in all computations. The nitric oxide concentration above 80 km may be considered reasonably well known, probably to within a factor of two. Below that altitude, the chemistry is uncertain and the effects of reactions such as

R54, R55 and R60 have not been studied thoroughly. Stroebel (1972) shows that values lower than those obtained by Meira (1971) are possible and suggests using limits obtained from electron densities in the D region. Figure II-1 shows nitric oxide concentrations used here as a basis for predicting infrared radiance at high altitudes, and is based on Stroebel's calculations.

Water vapor abundances are much less well known. There is general agreement that water vapor is present in the upper stratosphere in amounts of between 2 and 10 parts per million, Anderson (1971a); but the exact amount is unknown. Anderson (1971a, 1971b) has determined OH abundances from observation of fluorescent scattering of solar ultraviolet radiation. The concentrations are about 5×10^6 molecules/cm³ between 45 and 70 km, with error limits of about 120 per cent. Anderson's first paper includes a steady state photochemical model with diffusion and he uses this to infer a water vapor abundance of about one to two parts per million at 85 km. The calculations with the chemistry model described above assumed an initial concentration of three parts per million and were not run long enough to reach diurnal equilibrium. In addition, the eddy diffusion coefficients above 50 km, taken from Keneshea and Zimmerman (1970), are larger than the upper limit deduced by Anderson (1971a). It was decided to use them, however, because M. B. McElroy (private communication, 1972) has informed us that there has been an unpublished measurement of Reaction R12 which gives a value 2×10^{-10} cm³/sec which may lead to lower OH concentrations for a given water vapor abundance. The adopted water vapor abundances are given in Figure II-2, and are based on the (incomplete) chemistry program results.

While ozone abundances below about 50 km must take into account lateral transport as well as vertical transport by eddy mixing and molecular diffusion, photochemical models are adequate above that altitude, and agree with observations obtained by measuring absorption of solar and stellar

Nitric Oxide Concentration Profiles

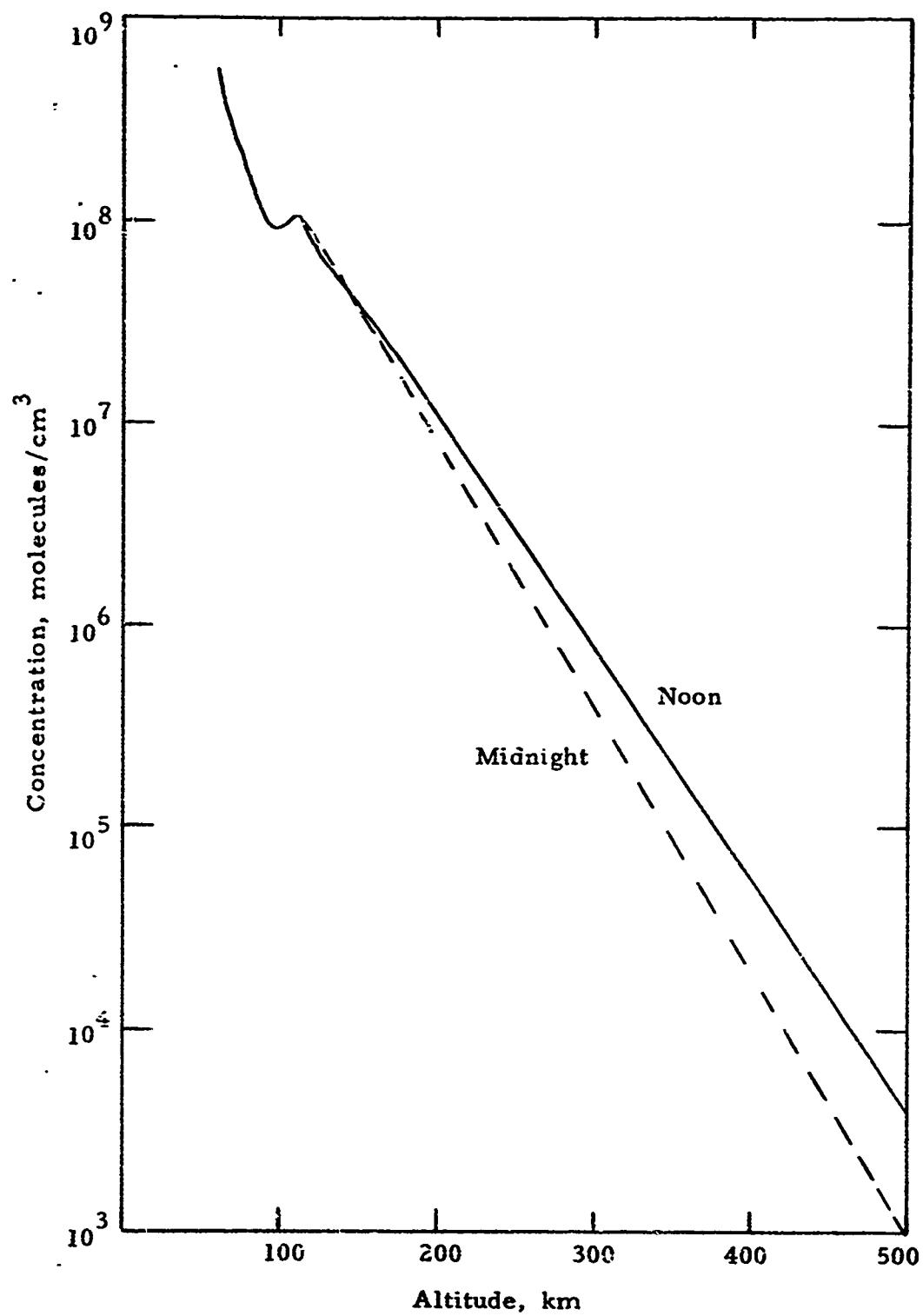


FIGURE II-1

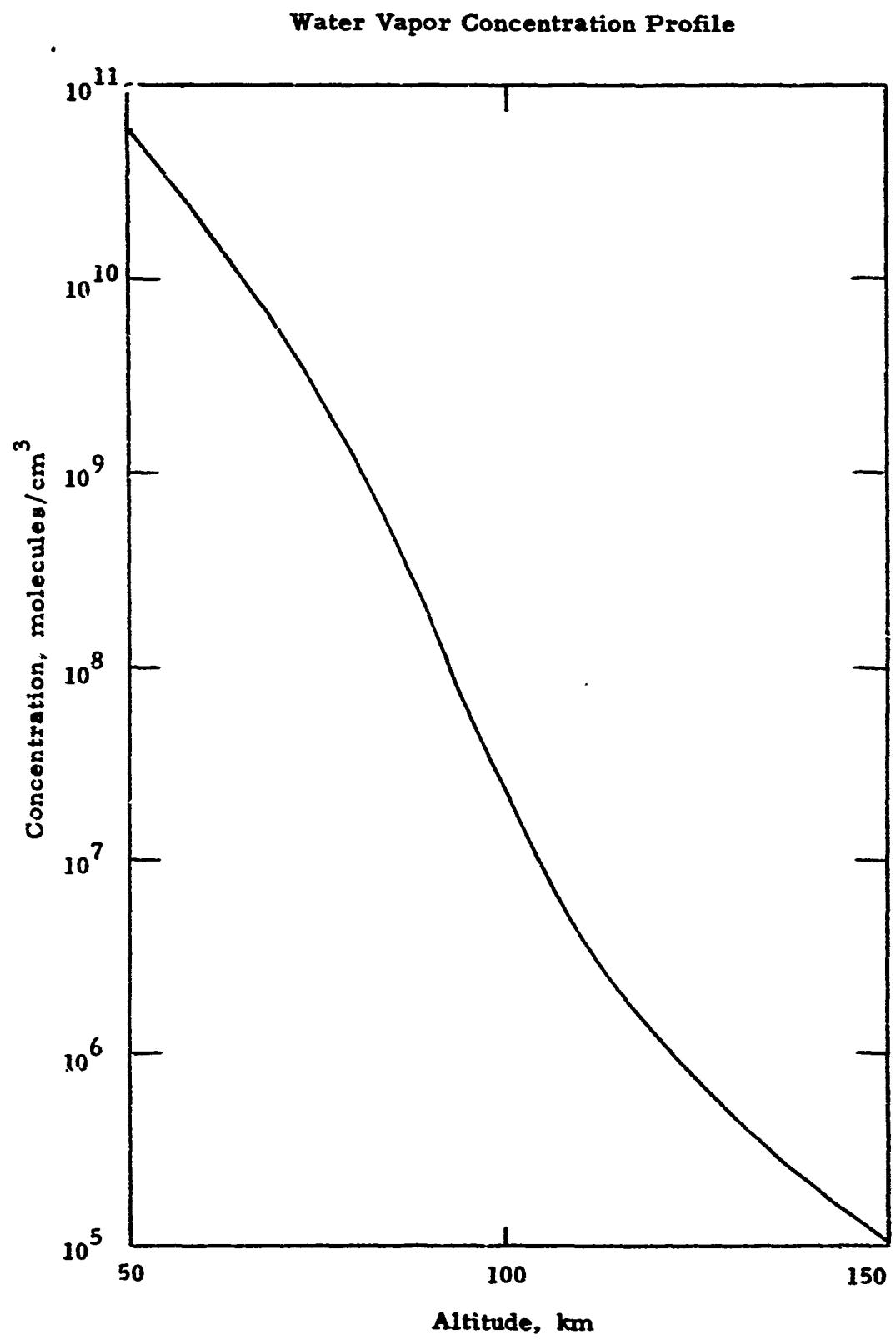


FIGURE II-2

ultraviolet radiation and those deduced from measurements of the molecular oxygen $1.27 \mu\text{m}$ infrared atmospheric band. The exact profile depends on assumed eddy diffusion coefficients, however, principally through atomic hydrogen and oxygen concentration. O_3 abundances used here are shown in Figure II-3, and were obtained from the chemistry program.

Carbon dioxide has a lifetime of about 10 days at the top of the atmosphere, where it is dissociated by solar radiation. It is well shielded by molecular oxygen below about 120 km, however, and should remain well mixed below 100 km. The only good measurement above 100 km is that of Offerman and von Zahn (1971), who find that between 120 and 140 km the mixing ratio is not more than 50 per cent less than the tropospheric value. Above 140 km, molecular diffusion is rapid enough compared to photodissociation to maintain diffusive equilibrium. While Hays and Olivero (1970) have obtained a rapid falloff in mixing ratio above 80 km, their results are incorrect because they neglect recombination by Reactions R33 and R34 above 70 km. While the chemistry program was not run long enough to reach realistic values of carbon dioxide concentrations, the profile shown in Figure II-4, based in part on Offerman and von Zahn (1971) should be adequate as a basis for computation of infrared radiances.

Although included in the chemistry program, methane is not considered as an important source of infrared radiation above 50 km, as it is destroyed by photodissociation and reaction with atomic oxygen and OH faster than it can be transported upward.

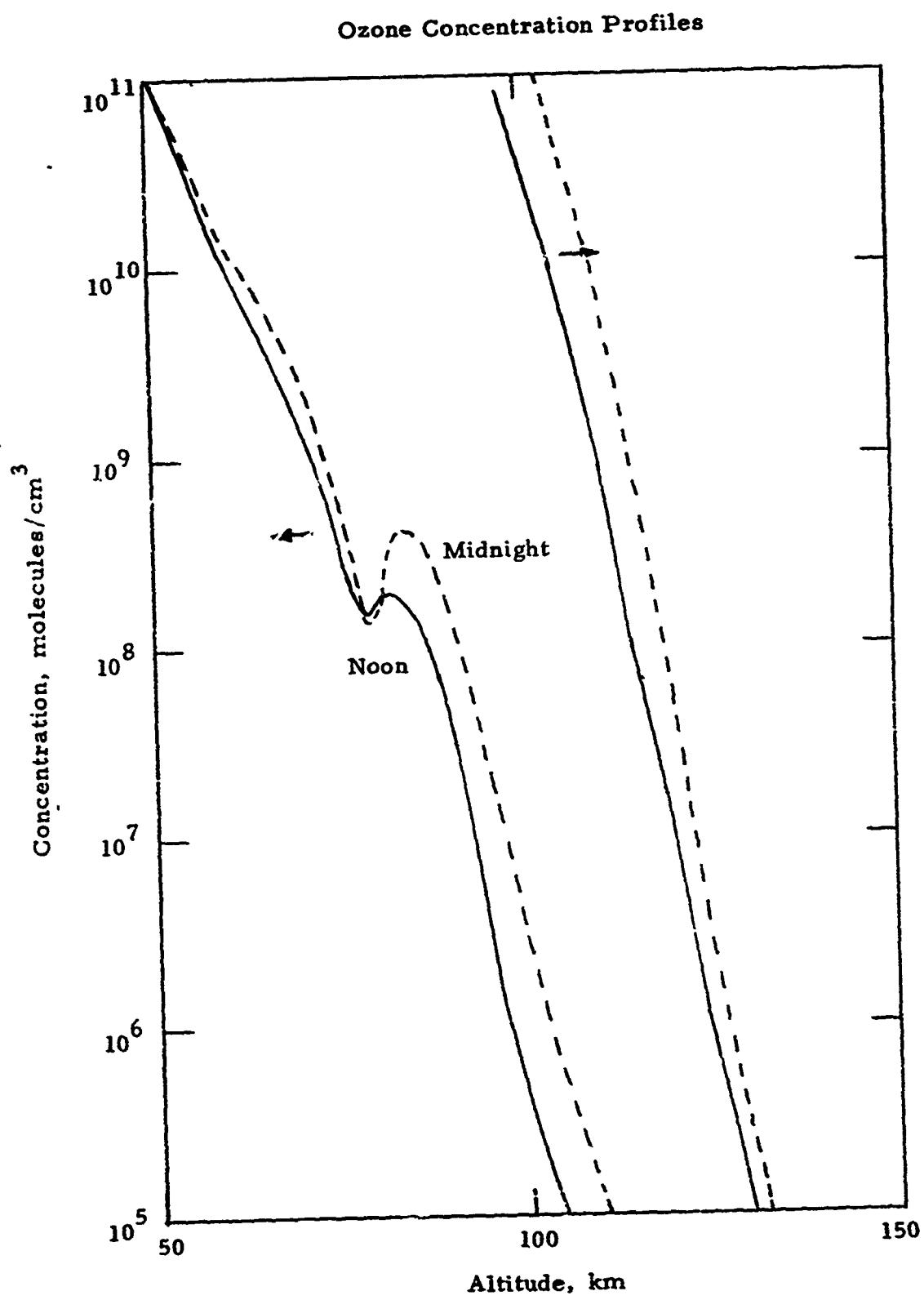


FIGURE II-3

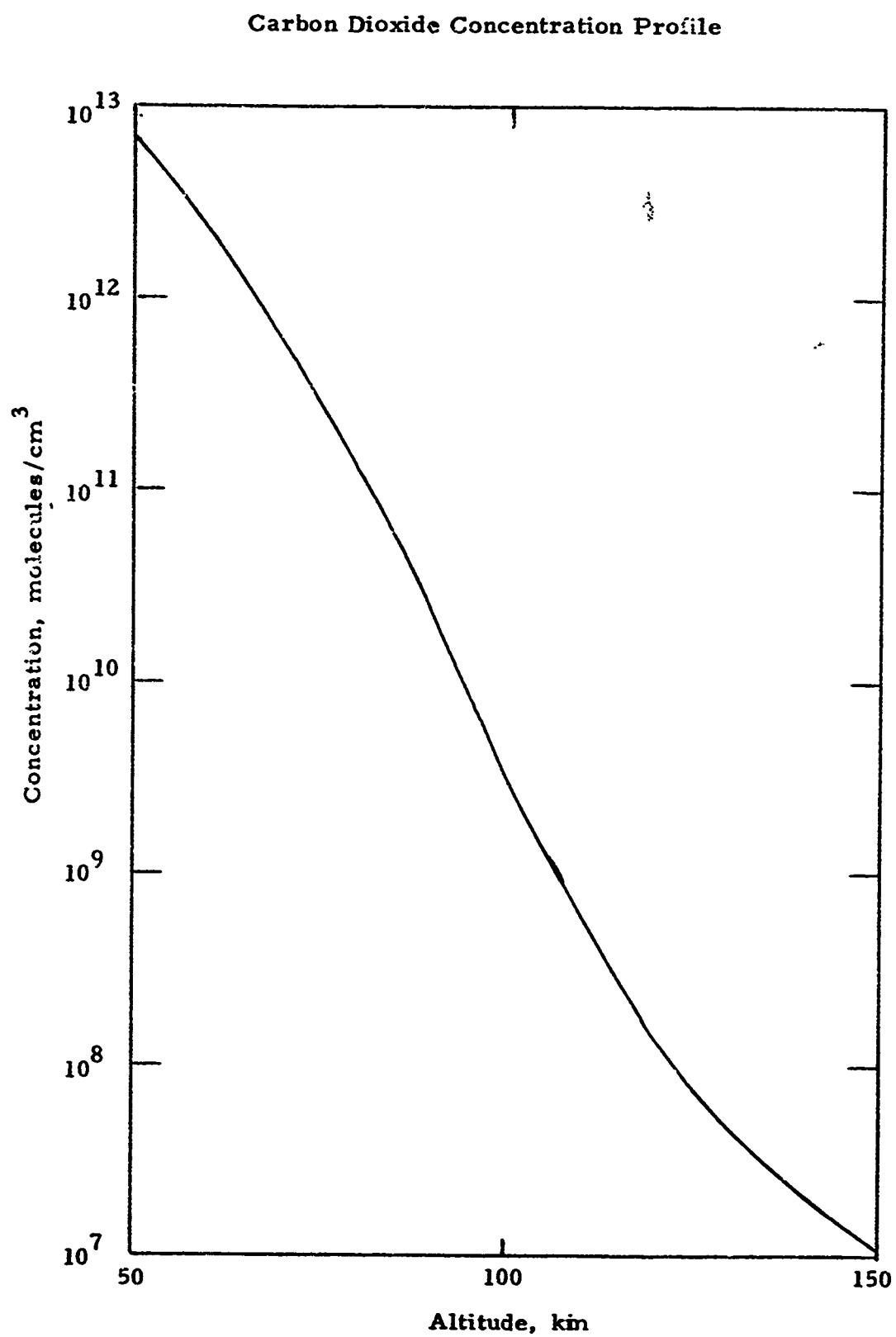


FIGURE II-4

SECTION III

EXCITATION MECHANISMS

A. General Considerations

Except for the pure rotational radiation from molecules such as water, the degree of excitation of vibrational levels determines the radiation from infrared emitting molecules. The physical processes affecting the population of vibrational states includes collisional excitation, radiative excitation by resonant absorption or fluorescent decay, chemical formation in a vibrationally excited state, and radiative and collisional de-excitation.

In the troposphere and lower stratosphere collisional excitation of vibrational levels is sufficiently rapid to compensate for radiative de-excitation, and vibrational populations are in thermodynamic equilibrium with translation and rotation. At altitudes above 30 to 50 km, however, radiative processes assume a dominant role in determining vibrational populations. Resonant scattering and fluorescent mechanisms become the dominant processes producing infrared radiation. At wavelengths greater than $5 \mu\text{m}$, the most intense source of radiation is the thermal emission from the earth's surface and from carbon dioxide, water vapor and ozone present at lower levels in the atmosphere. During the day, the effects of solar radiation must be included since fluorescent processes may lead to significant excitation of vibrational states. At wavelengths shorter than $6 \mu\text{m}$, resonant absorption of solar infrared flux maintains vibrational temperatures above 200 K.

The following parts of this section discuss vibrational excitation and de-excitation and the model developed for computation of radiative processes.

B. Collisional Excitation

In computing radiances at high altitudes, it must be recognized that vibrational levels are not populated at thermal equilibrium values. Radiation de-populates vibrational states rapidly and collisional excitation is not sufficiently efficient to maintain a Boltzmann distribution of vibrational states. Collisional excitation and de-excitation rates are required to compute the balance of opposing mechanisms which determine actual vibrational populations.

Four collisional processes are considered which affect the vibrational state of a molecule. (1) translational-vibrational (T-V) interactions in which translational energy is transformed into vibrational energy or vice-versa during a collision, (2) intermolecular vibrational exchange (V-V) in which a molecule of one species exchanges a quantum of vibrational energy with a molecule of another species, (3) intramolecular vibrational exchange in polyatomic molecules in which a collision transfers the energy in one mode of vibration into another mode within the same molecule, and (4) collisions between an atom and molecule in which there is either atom exchange or the formation of a collision complex which has a lifetime long enough to equilibrate kinetic and vibrational temperatures. This latter process may be considered a special case of the first mechanism.

When a molecule in the ground state collides with another molecule there is a finite probability P_{VT} that a portion of the relative translational energy will be transformed to vibrational energy if the translational energy is equal to or exceeds the vibrational energy. Similarly, if the molecule is in an excited vibrational state, there is a finite probability P_{TV} that the vibrational energy will be converted to relative translational energy during the collision. For a Boltzmann distribution of translational energies at a given temperature,

$$P_{TV} = P_{VT} \frac{g_u}{g_l} \exp\left(-\frac{hc}{\lambda_0 kT}\right) \quad (3-1)$$

Similar expressions hold for intermolecular and intramolecular V-V transfer.

The rate at which a vibrational level is excited (k_{TV}) or de-excited (k_{VT}) is given by the product of the collision frequency Z and the transition probability. Experimental determinations of collisional excitation rates may be reported as probabilities, excitation rates or relaxation times. The latter are related to excitation and de-excitation rates by (Herzfeld and Litovitz, 1959)

$$\frac{1}{\tau} = k_{VT} + k_{TV} \quad (3-2)$$

Excitation rates depend on temperature and number density through the strong temperature variation of the transition probability and the square root temperature and linear density variation of the collision frequency.

The most important molecular collision partners in the atmosphere are nitrogen and oxygen, and a knowledge of their vibrational temperatures and effects is important. These will be treated first and followed by a brief discussion of the relative importance of collisional excitation mechanisms for nitric oxide.

Vibrationally excited oxygen can be produced in the atmosphere by recombination of atomic oxygen



by formation from ozone



by fluorescence in the discrete Schumann-Runge band system



by transfer of kinetic energy to vibrational energy



by electron impact



by exchange of vibrational quanta with molecular nitrogen (and other molecules)



and by the strong collisional interaction with atomic oxygen



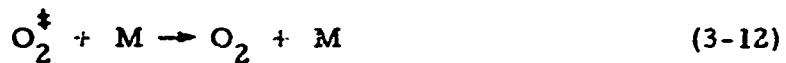
Vibrationally excited oxygen can be quenched by the strong collisional interaction with atomic oxygen



by transfer of vibrational quanta to molecular nitrogen (and other molecules)



and by transfer of vibrational energy to kinetic energy



Above the mesopause, and up to 300 km, reactions (3-9) and (3-10) dominate production and loss of vibrational excitation and can be shown to maintain vibrational distributions close to thermal equilibrium values.

Bates and Moiseiwitsch (1956) proposed that the atom exchange reaction



is sufficiently rapid in quenching vibrationally excited oxygen that the reaction proposed by Krassovsky (1955)



cannot be important in the production of vibrationally excited OH. Bauer and Tsang (1963) suggested that reaction (3-14) would be important in relaxing the

vibrational levels of shock heated oxygen and estimated the rate coefficient to be about $2 \times 10^{-10} \exp(-8000/RT) \text{ cm}^3/\text{sec}$.

The rate for atom exchange reaction (3-14) has been measured near room temperature by Ogg and Sutphen (1953, 1954), Brennan and Niki (1965), Jaffe and Klein (1966) and Herron and Klein (1964). Johnston (1968) has reviewed these results and recommends a value of $10^{-12} \text{ cm}^3/\text{sec}$ for the rate coefficient at 273 K. Garnett, Kistiakowski and O'Grady (1969) have measured the rate coefficient near 1800 K. Clark, Garnett and Kistiakowski (1970) have combined the latter results with those of Jaffe and Klein (1966) to suggest a temperature dependence given by

$$\text{r}_{13} = 10^{-12.48 \pm 0.3} T^{1/2} \exp[-(960 \pm 700)/RT] \text{ cm}^3/\text{sec} \quad (3-15)$$

Kiefer and Lutz (1967) have measured the vibrational relaxation time of molecular oxygen in the presence of atomic oxygen at temperatures between 1600 and 3300 K. They find that over this temperature range the product of pressure P and relaxation time τ_{O_2} is given by

$$P\tau_{O_2} = (4.35 \pm 0.19) \times 10^{-8} - (7.75 \pm 0.81) \times 10^{-12} T \text{ atm-sec} \quad (3-16)$$

The prediction of Bauer and Tsang (1963) agrees with this result within a factor of two. The rate coefficient for atom exchange from Equation (3-15) is $9.8 \times 10^{-12} \text{ cm}^3/\text{sec}$ at 1600 K and the de-excitation rate coefficient derived from Equation (3-16) is $8.6 \times 10^{-12} \text{ cm}^3/\text{sec}$ at 1600 K. The close agreement

supports the assumption used here that the vibrational de-excitation rate is within a factor of two of the atom exchange rate, which may be considered well determined.

Further evidence is given by the theoretical computation of Breig (1969) who estimated the rate of de-excitation of high vibrational levels of molecular oxygen by reaction with atomic oxygen. He obtains total reaction rates of the $V = 5$ and $V = 25$ levels at 200 K. Breig's (1969) results may be used as a qualitative argument for the further assumption that higher vibrational levels of molecular oxygen will reach steady state populations in times of the order of that required by the $V = 1$ level.

Dalgarno (1963, 1967, 1970) has suggested that fluorescence in the discrete Schumann-Runge band system may be an important source of vibrationally excited oxygen in the mesosphere and thermosphere. The experimental results of Ackerman, Biaume and Nicolet (1969) and Hudson and Carter (1969) indicate that excitation to $V' > 3$ results in predissociation rather than fluorescence. If this conclusion is accepted, the only transition of importance is the $(2, 0)$ transition at 1971 \AA . This has an oscillator strength f in absorption of 2.34×10^{-4} according to the computations of Nicholls (1964). The solar flux πF_o at 1971 \AA is about 1.2×10^{11} photons/($\text{cm}^2 \text{-sec-} \text{\AA}$) according to Detwiler, et al. (1961) or 1.4×10^{11} photons/($\text{cm}^2 \text{-sec-} \text{\AA}$) according to Ackerman (1970). At the top of the atmosphere, the absorption rate g per oxygen molecule in the $(2, 0)$ band is 9.6×10^{-7} photons per second from the relation

$$g = \frac{\pi e^2}{mc^2} \pi F_o f \lambda^2 \quad (3-17)$$

Using the Einstein A coefficients given by Nicholls (1964), it is found that the mean vibrational level following fluorescent emission is 11 so that about 10^{-5} vibrational quanta are produced each second per molecule.

The effective rates of vibrational excitation by electron impact may be determined from the electron cooling rates computed by Lane and Dalgarno (1969). Using the electron densities and temperatures observed by Spencer, et al. (1965), typical rates are 3.3×10^{-6} , 1.8×10^{-5} and 6.2×10^{-5} excitations per molecule per second at 150, 200 and 300 km, respectively.

The effects of the above processes on molecular oxygen vibrational temperatures were computed for the CIRA 1965 mean atmosphere for altitudes between 80 and 300 km. The rate coefficients given by Johnston (1968) were used for three body recombination of atomic oxygen and for the reaction of atomic oxygen with ozone. The maximum possible vibrational excitation of the products was assumed. The rate coefficients given by Gilmore, Bauer and McGowan (1969) were used for vibrational excitation by collisional transformation of kinetic energy and collisional exchange of vibrational quanta with molecular nitrogen. The de-excitation rate by reaction with atomic oxygen was taken to be $3.3 \times 10^{-13} T^{1/2} \exp(-485/T) \text{ cm}^3/\text{sec}$, the mean value suggested by Clark, Garnett and Kistiakowski (1970).

Even with the upper limits to nitrogen vibrational temperatures given by Walker, Stolarski and Nagy (1969) the rate of vibrational excitation of molecular oxygen by collisional transfer of energy with nitrogen is less than 10^{-6} excitations per molecule per second at any altitude above 80 km.

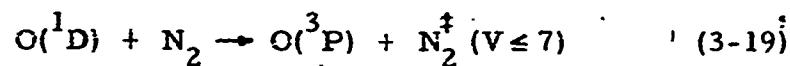
At all altitudes below 200 km, the vibrational population of molecular oxygen as computed is within two per cent of the thermal equilibrium value. At 300 km, excitation by electron impact increases the population of the first vibrational level by less than twenty per cent. Thus, at all altitudes where

polar molecules will be significantly excited by molecular oxygen, the vibrational temperature may be taken to be the kinetic temperature. This result agrees with the conclusions of Bauer, Kummier and Bortner (1971).

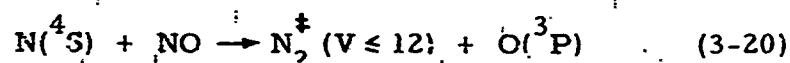
The vibrational temperature of molecular nitrogen at high altitudes remains uncertain. The principal processes which have been suggested to produce vibrationally excited nitrogen are transfer of kinetic energy to vibrational quanta



quenching of $O(^1D)$ by collision



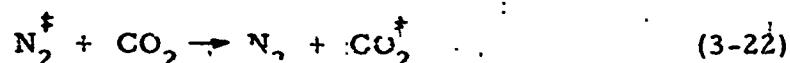
reaction of atomic nitrogen and nitric oxide



and excitation by electron impact



The principal process which quenches vibrationally excited nitrogen is collisional transfer of vibrational quanta to the ν_3 vibrational mode of carbon dioxide



Reaction (3-18) is insignificant above 70 or 80 km. If all the available energy were transformed to vibrational excitation, quenching of O(¹D) would be the most important process above 80 km. However, Fisher and Bauer (1970) estimate that the process is only about five per cent efficient and Black and Eckstrom (1971) have obtained an experimental efficiency of 8.3 ± 6.5 per cent. Above 120 km, reaction (3-20) is the most important source of excitation, Morgan, et al. (1962) and Morgan and Schiff (1963) having determined that about one-third of the available energy goes into vibrational excitation. Reaction (3-21) is nearly as an important source, the electrons involved being those produced by photo-ionization in the E-region.

Walker (1968) and Walker, Stolarski and Nagy (1969) have computed theoretical estimates of nitrogen vibrational temperatures. The first paper neglected collisional transfer of vibrational energy to carbon dioxide and obtained an approximately constant vibrational temperature of 3000 K above 110 km. Corbin, et al. (1970) noted that this result was too high near 110 km, more energy being transferred to carbon dioxide than could be produced by the assumed excitation mechanisms. The second paper included quenching by carbon dioxide and recognized that the O(¹D) excitation mechanism might be inefficient. Results were given for zero and 100 per cent excitation by this mechanism. The first assumption gives a maximum vibrational temperature of 1700 K at 300 km. The vibrational temperature is below 1000 K at all times for altitudes below 140 km. Minimum vibrational temperatures occur at dawn and rise steadily until sunset. Using these results, it is found that except for carbon dioxide band emissions originating from the ν_3 mode, excess vibrational excitation of nitrogen is unimportant for radiation emitted by the molecules studied here.

Degges (1971) has discussed the mechanisms which contribute to

vibrational excitation of nitric oxide. He proposes that above 80 km, the most important collisional process is the atom exchange mechanism



Using the low temperature measurement of Herron and Klein (1964) and an argument based on the adiabatic correlation diagram of Donovan and Husain (1970) and the temperature dependence of the similar atom exchange reaction of atomic oxygen with carbon monoxide, he suggests that the de-excitation rate of vibrationally excited nitric oxide by collision with atomic oxygen lies between $10^{-13} T^{1/2} \text{ cm}^3/\text{sec}$ and $5 \times 10^{-13} T^{1/2} \exp(-1000/RT) \text{ cm}^3/\text{sec}$. The latter rate has been adopted in the present computations. Figure III-1 compares the effect of this process with exchange of vibrational quanta with molecular oxygen and nitrogen. Even if the nitrogen vibrational temperature is 2000 K, nitrogen is a less efficient collision partner above 120 km.

The rates used for other vibrational excitation processes are largely the same as those used by Corbin, et al. (1969). Vibrational exchange rates between nitric oxide and nitrogen are those measured by Basco, et al. (1961, 1962) with the temperature dependence given by Gilmore, et al. (1969) which is based on the correlation scheme of Millikan and White (1963). Collisional excitation rates used for carbon dioxide and water vapor are taken from the review of Taylor and Bitterman (1969), with the addition of the experimental results of Stephenson et al. (1971) on intramolecular vibrational exchange in carbon dioxide. The rates used for nitrous oxide are those of Yardley (1968) and Simpson, et al. (1968). Estimated rates for ozone excitation were obtained by use of Millikan and White's (1963) correlation scheme, and comparison with other systems. Because of the lower temperatures at the mesopause (about 80 to 90 km) and the rapid decrease in number density with altitude, the only critical rates above 80 km are the oxygen atom exchange with nitric oxide and the vibrational exchange between carbon dioxide and molecular nitrogen.

Nitric Oxide Collisional Excitation Rates

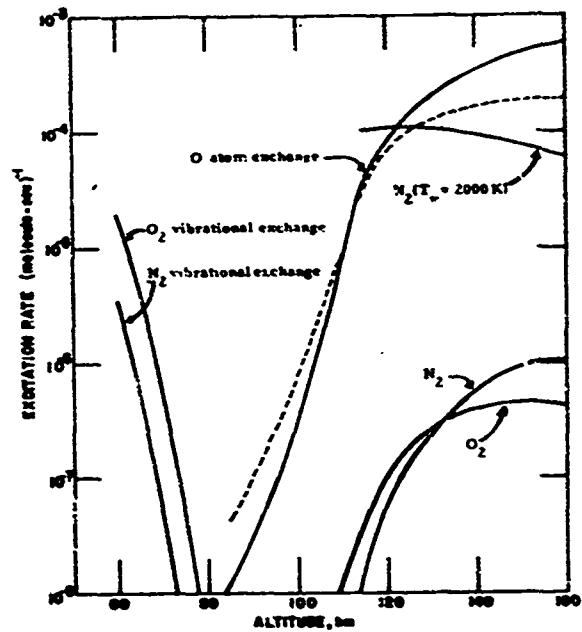
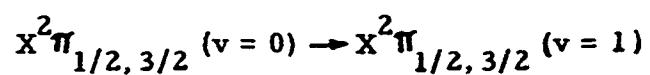


FIGURE III-1

C. Radiative Processes and Modeling

The physical processes and assumptions used in developing a model for transport of infrared radiation in the upper atmosphere are discussed below, beginning with the interaction of electromagnetic radiation with an isolated atom or molecule. An understanding of the basic processes involved is the first step in any computation of the radiation from a gas or mixture of gases. Subsequently, absorption from a continuum source, a spectrally varying source and fluorescent processes is treated. The effects of optical thickness when the path of the radiation includes a large number of molecules of the same species is considered for spectral lines with Doppler shape. Finally, a model for the transport of radiation for a single vibration-rotation band is described.

When treating a problem in which the number of photon emitted or absorbed by an atom or molecule must be considered rather than total energy emitted, it is convenient to examine the physics of the interaction of radiation with matter through use of the Einstein A and B coefficients. In treating a radiative problem such as the current study of high altitude infrared radiances which involves transfer of energy between molecules through collisions, this approach is a necessity. In the following discussion, cgs units are used except where explicitly stated.

The Einstein A_{ul} coefficient is the rate at which an atom or molecule in an excited state spontaneously emits radiation. It has the units photons/sec-molecule. In an assemblage of molecules all in a state given by the Einstein A_{ul} coefficient for the particular radiative transition from a state of higher energy (subscript u) to one of lower energy (subscript l).

In addition to spontaneous emission, two other processes occur. These are absorption, characterized by the Einstein coefficient for absorption B_{lu} ,

and induced emission, characterized by the Einstein coefficient for induced emission B_{ul} . In a radiation field with spectral density, $\rho_{\nu_{lu}}$, the probability that an atom or molecule absorbs a quantum of radiation in unit time is $B_{lu}\rho_{\nu_{lu}}$. When radiation density is expressed in c. g. s. units ergs-sec/cm³, the coefficient B_{lu} has units cm³/ergs-sec. Similarly, an atom or molecule in a radiation field with the above spectral density and in an excited state emits radiation at the rate $B_{ul}\rho_{\nu_{lu}}$ in addition to that characterized by the coefficient A_{ul} . The Einstein coefficients are properties of an atom or molecule. If one coefficient is known, the others may be determined by the relations

$$A_{ul} = 8\pi h B_{ul} / \lambda^3 \quad (3-24)$$

and

$$g_l B_{lu} = g_u B_{u_l} \quad (3-25)$$

Thus, it is possible to treat the problem knowing only the Einstein A_{ul} coefficient.

Experimental determinations of the interaction of infrared radiation with gases are usually made by measurements of light absorption. Experimental results may be expressed as integrated absorption from a continuum source,

$$S'_{lu} = N_l \frac{A_{ul} \lambda_{lu}^2}{8\pi} \frac{g_u}{g_l} \left[1 - \exp \left(-\frac{hc}{\lambda_{lu} kT} \right) \right] \quad (3-26)$$

or as line or band strengths

$$S_{lu} = S'_{lu}/pc \quad (3-27)$$

In the visible and ultraviolet regions of the spectrum, it is customary to use oscillator strengths to characterize the interaction of radiation and matter. In this case, the defining equation is

$$S'_{lu} = \frac{\pi e^2}{mc} N_l f_{lu} \left[1 - \exp \left(-\frac{hc}{\lambda_{lu} kT} \right) \right] \quad (3-28)$$

The results of theoretical computations of the interaction of matter with radiation are frequently expressed as dipole moments, μ_{ul} . These are related to the Einstein A coefficient by

$$A_{ul} = \frac{64\pi^4}{3h\lambda^3} \frac{g_u}{g_l} |\mu_{ul}|^2 \quad (3-29)$$

The rate at which a single atom or molecule absorbs and reradiates light from a parallel beam from a continuum source at a wavelength λ_o corresponding to a resonance transition is (Mitchell and Zemansky, 1961):

$$\begin{aligned} G &= \frac{\pi e^2}{mc^2} I_{oo} f_o \lambda_o^2 && \text{(photons/sec)} \\ &= 8.852 \times 10^{-13} I_{oo} f_o \lambda_o^2 && \text{(photons/sec)} \end{aligned} \quad (3-30)$$

where I_o is the continuum source flux and f_o is the oscillator strength. If the incident flux is expressed in photons/cm²·μm, and oscillator strength is replaced by the equivalent line or band strength S expressed as cm⁻² atm⁻¹,

$$G = 3.72 \times 10^{-24} I_o S \lambda^2 \quad (3-31)$$

Implicit in this expression is the convenient relation between the Einstein A_{ul} coefficient and line or band strength with wavelength dimensions μm

$$A_{ul} = 2.804 S(\text{cm}^{-2} \text{atm}^{-1}) / \lambda^2 (\mu\text{m}) \quad (3-32)$$

When the source is an extended black body surface with a spectral radiance N_λ , the G factor is obtained by integration over the solid angle subtended by the source. For radiation from a plane parallel surface of infinite extent,

$$G = 1.169 \times 10^{-23} N_\lambda S \lambda^2 \quad (3-33)$$

Another purely radiative mechanism of importance in upper atmosphere radiance computations is fluorescence. A striking example occurs for the weak 10.4 μm CO₂ band. Absorption of solar radiation by CO₂ 4.3 μm band maintains the ν₃ vibrational mode at a vibrational temperature of about 290 K. During the day, this leads to an enhancement of emission in the

10.4 μm band by as much as two orders of magnitude when viewed along the earth's limb from outside the atmosphere.

Fluorescence occurs when the upper state of the resonance transition reradiates into other than the initial states. The relative probability of a radiative transition to a lower state, n from the upper state, u when there are k possible lower states is:

$$P_{un} = \frac{A_{un}}{\sum_{j=1}^k A_{uj}} \quad (3-34)$$

where the A_{uj} are the Einstein A coefficients for the spontaneous emission probabilities for a transition from the upper state to the j th lower state.

In the case of molecular resonance-fluorescent scattering at low temperature, only the lowest vibrational level ($v'' = 0$) in the ground electronic state is populated significantly. Absorption of a photon excites the molecule to a vibrational level, v' in the same or a higher electronic state. Radiation is possible from this state to the initial level ($v'' = 0$) or to other vibrational levels ($v'' \neq 0$) in the ground electronic state. The rate of resonance fluorescent scattering in a given electronic vibrational transition may be obtained by combining Equations (3-30) and (3-34) and introducing appropriate subscripts:

$$G_{v'v''} = 8.853 \times 10^{-17} I_{v'0} f_{v'0} \lambda_{v'0}^2 \frac{A_{v'v''}}{\sum_{v''} A_{v'v''}} \quad (3-35)$$

Here the subscript $v'v''$ refers to a transition from an upper state with vibrational level v' to a lower state with vibrational level v'' . The subscript $v'o$ refers to absorption of a photon by a molecule in the lowest vibrational level of the ground state, exciting the molecule to a vibrational level v' in the same or a higher electronic state.

In developing a realistic model of the interaction of radiation with matter, it is necessary to take into account the details of absorption. Line shape must be considered because it determines the amount of radiation escaping from an optically thick layer of gas. Thus, for large optical thicknesses (greater than a magnitude of about 10), the total emission from an isolated spectral line with Lorentz shape is proportional to the square root of the optical thickness, while that from a line with Doppler shape is proportional to the square root of the logarithm of the optical thickness. In addition, absorption of radiation emitted at one place in the gas by a molecule at another location cannot be computed without knowledge of the line shape.

At high altitudes, the profile of the spectral absorption curve of an individual line in a vibration-rotation band is predominantly due to velocity or Doppler broadening. Kuhn and London (1969), who investigated the heat budget of the atmosphere between 30 and 110 km, report that radiative transfer calculations require the use of the Voigt profile (including both collisional and Doppler broadening) at altitudes between 20 and 70 km. Alternatively, the Doppler profile is adequate at higher altitudes where the Doppler shape is the largest contributor to line broadening. The basic computational model therefore assumes a Doppler profile.

In addition to the use of Doppler shape for a single line, several other assumptions have been made about the radiative transfer within lines of a band. These are the following:

- (1) Rotational levels within a vibrational level remain in equilibrium with the translational temperature. This is valid up to at least 150 km according to Goody (1964).
- (2) There is complete redistribution of frequency within a single line following absorption of radiation.
- (3) There is complete redistribution of absorbed energy among all rotational levels.
- (4) Line strengths are used as if each line were at the band center, neglecting wavelength variation across a band.
- (5) There is no overlap of adjacent lines.
- (6) Temperature variations at different levels do not affect the radiative transfer. This assumption probably constitutes the largest source of error in computing transmission.

The major result is to make computed band radiances too small when determining escape of radiation from a warm layer overlaid by a cooler layer.

The above assumptions lead to the following treatment, which begins with consideration of a single line and from this develops the method used for treating radiative transfer in an entire band. The spectral absorption coefficient of a Doppler broadened line is (Mitchell and Zemansky, 1961):

$$k(\nu) = \frac{1}{\Delta\nu_D} \sqrt{\frac{\ln 2}{\pi}} \frac{\pi e^2}{mc} N_{1,0} \exp \left[-\left(\frac{\nu - \nu_0}{\Delta\nu_D} \sqrt{\ln 2} \right) \right] \quad (3-36)$$

where the Doppler half width at half maximum is

$$\Delta\nu_D = \sqrt{\frac{2RT \ln 2}{Mc^2}} \nu_0 \text{ (sec}^{-1}\text{)}$$

The amount of light absorbed by the line per unit frequency interval is

$$\begin{aligned} I(\nu) A(\nu) d\nu &= I(\nu) (1 - T(\nu)) d\nu \\ &= I(\nu) (1 - e^{-k(\nu)}) d\nu \end{aligned} \quad (3-37)$$

and the total light absorbed is

$$\begin{aligned} \int_0^\infty I(\nu) A(\nu) d\nu &= \int_0^\infty I(\nu) (1 - T(\nu)) d\nu \\ &= \int_0^\infty I(\nu) (1 - \exp \left\{ -K_0 \exp \left[-\left(\frac{\nu - \nu_0}{\Delta\nu_D} \ln 2 \right)^2 \right] \right\}) d\nu \end{aligned} \quad (3-38)$$

where the integration is over all frequencies and

$$\kappa_o = \frac{1}{\Delta\nu_D} \sqrt{\frac{\ln 2}{\pi}} \frac{\pi e^2}{mc} N_1 f_o$$

The line will absorb only near the center frequency ν_o and $I(\nu)$ may be replaced by $I(\nu_o)$. Making the substitution

$$w = \frac{\nu - \nu_o}{\Delta\nu_D} \sqrt{\ln 2}$$

$$\int_0^\infty I(\nu) A(\nu) d\nu = I(\nu_o) \frac{\Delta\nu_o}{\sqrt{\ln 2}} \int_{-\infty}^\infty \left(1 - e^{-\kappa_o e^{-w^2}} \right) dw$$

$$= I(\nu_o) \frac{\pi e^2}{mc} N_1 f_o \left(1 - \frac{\kappa_o}{2! \sqrt{2}} + \frac{\kappa_o^2}{3! \sqrt{3}} + \dots \right) \quad (3-39)$$

The corresponding expression on a wavelength basis is

$$\begin{aligned} \int_{-\infty}^\infty I(\lambda) A(\lambda) d\lambda &= I(\lambda_o) \frac{\pi e^2}{mc} N_1 f_o \lambda_o^2 \left(1 - \frac{\kappa_o}{2! \sqrt{2}} + \frac{\kappa_o^2}{3! \sqrt{3}} + \dots \right) \\ &= I(\lambda_o) \kappa_o \left(1 - \frac{\kappa_o}{2! \sqrt{2}} + \frac{\kappa_o^2}{3! \sqrt{3}} + \dots \right) \\ &= G N_1 \left(1 - \frac{\kappa_o}{2! \sqrt{2}} + \frac{\kappa_o^2}{3! \sqrt{3}} + \dots \right) \end{aligned} \quad (3-40)$$

The quantity in parentheses in Equation (3-40) is simply a factor by which the product of G and N_1 must be multiplied to account for the effects of total optical thickness κ_o in computing the total absorption of radiation by a column containing N_1 molecules/cm² in the lower state. This quantity is termed S by Mitchell and Zemansky (1961) who present tabulations of its value. Penner (1959) gives an asymptotic expansion for large values of κ_o . The astrophysical literature frequently uses the notation

$$L(\kappa_o) = \kappa_o S(\kappa_o) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \left(1 - e^{-\kappa_o e^{-w^2}} \right) dw \quad (3-41)$$

The factor by which G must be multiplied to obtain the true rate of absorption at an optical depth κ_o may be found by differentiating Equation (3-41) with respect to κ_o (Ivanov and Shcherbakov, 1965):

$$M_1(\kappa_o) = \frac{dL(\kappa_o)}{d\kappa_o} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-w^2} - \kappa_o e^{-w^2} dw \quad (3-42)$$

The factor by which G must be multiplied to obtain the actual absorption from an extended black body source is (Ivanov and Shcherbakov, 1965)

$$N_1(\kappa_o) = \int_0^{2\pi} \int_0^{\pi/2} \cos \theta \sin \theta M_1 \left(\frac{\kappa_o}{\cos \theta} \right) d\theta \quad (3-43)$$

When the source of radiation is a Doppler profile exactly that of the absorbing line, the differential absorption at optical thickness κ_0 is given by

$$M_2(\kappa_0) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-2w^2 - \kappa_0^2 - w^2} dw \quad (3-44)$$

and G must be multiplied by this factor. Also, if the source is an infinite plane layer (not a surface) radiating with a Doppler profile, G must be multiplied by:

$$N_2(\kappa_0) = \int_0^{2\pi} d\phi \int_0^{\pi/2} M_2\left(\frac{\kappa_0}{\cos \theta}\right) \sin \theta d\theta \quad (3-45)$$

Corbin, et al. (1970) evaluated the functions of Equations (3-41) through (3-45) by numerical integration and obtained polynomial approximations for the entire range of variation of x_0 from zero to infinity, using the known asymptotic forms as a guide at large values. They then used these functions to compute the corresponding functions for vibration-rotation bands of linear molecules. The resulting functions are conveniently parameterized by using the optical thickness at the center of the strongest line of a band. It was found that two sets of such functions were adequate, one set for parallel transitions and one set for perpendicular transitions.

In extending the modeling to non-linear molecules, it was found to be more convenient to use the number of molecules in the line of sight as the

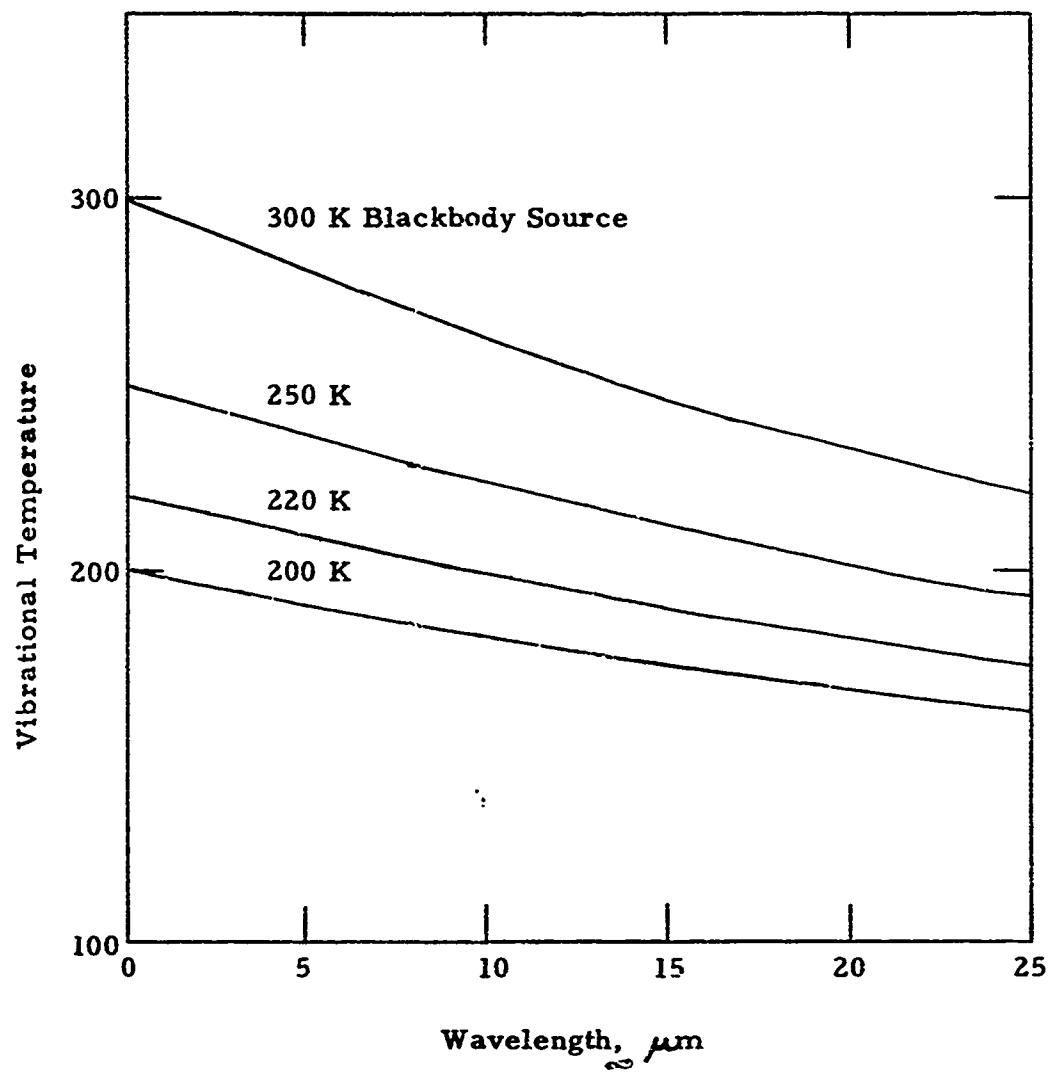
model parameter. Since upper atmosphere temperatures are near or below 250 K where optical thickness affects results, the functions used in the program for the water vapor ν_2 and ozone ν_1 and ν_3 bands were computer for a temperature of 250 K. Because ozone and water vapor are present in much smaller concentrations than carbon dioxide, the effects of optical thickness are much smaller.

At altitudes where collisional excitation rates are small, particularly between 80 and 100 km and above 120 km, the radiation from the lower atmosphere and the sun will control vibrational excitation of infrared emitting molecules. Figure III-2 shows vibrational temperatures which will be maintained by radiation from the earth's surface and lower atmosphere assuming that the upward radiation may be treated as originating from a blackbody at a given temperature. The effective temperature will vary with wavelength and lower atmosphere temperature and composition. Curves are drawn for blackbody temperatures of 200, 220, 250 and 300 K. Typical radiation temperatures between 5 and 25 μm lie between 190 and 310 K (E. G. Wark, et al., 1962). The main feature of importance in these curves is the decrease in vibrational temperature with increasing wavelength for a given blackbody temperature.

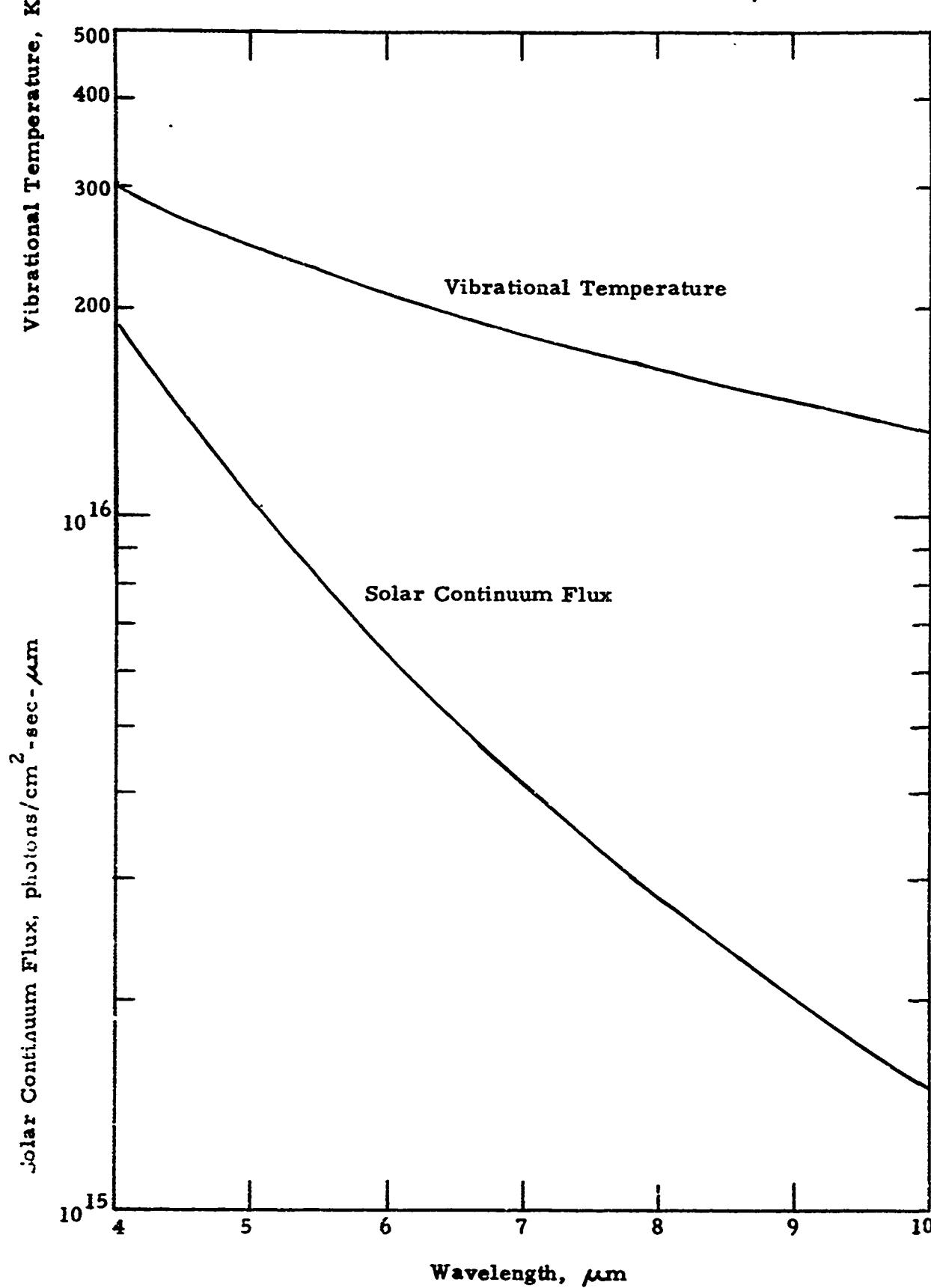
During the day, solar infrared flux is important in exciting the shorter wavelength transitions. Figure III-3 shows solar infrared fluxes at the top of the atmosphere given by Johnson (1964) and the resulting vibrational temperatures for a molecule at the top of the atmosphere. Absorption of radiation by molecules between the lower atmosphere radiation source or the sun decreases the effective incident radiation. This is partially, but not completely, offset by the radiation of these molecules.

The band functions are used to determine the effects of absorption between a molecule at a given altitude and the various sources of radiation affecting a

Vibrational Temperature of Molecule with
Excitation by Infinite Plane Blackbody Source
Alone Balanced by Spontaneous Emission,
0 to 25 μm



Solar Continuum Flux and Corresponding Vibrational Temperature of a Molecule at the Top of the Atmosphere, Excitation by Solar Flux Alone Balanced by Spontaneous Emission, 4 to 10 μm



given band in the following way. The vertical optical paths to the lower boundary and to each level in the atmosphere are computed and, for daytime conditions, the optical path to the assumed top of the atmosphere in the direction of the sun. The effective radiation from the lower boundary is determined by multiplying by the value of the band function $N_1^b(\kappa_o)$ corresponding to the line function of Equation (3-43). The effective radiation from the sun is determined by multiplying by the band function $M_1^b(\kappa_o)$ corresponding to the line function of Equation (3-42). Finally, the effective radiation from all atmospheric levels is obtained by integrating the product of emission at each level and the band function $N_2^b(\kappa_o)$, which corresponds to the line function of Equation (3-45). Vibrational populations are determined by balancing collisional and radiative excitation and de-excitation rates. Total band intensities at an observation point inside or outside the atmosphere are computed by determining the optical path from each level to the observation point and integrating the product of local emission rate and the band function $M_1^b(\kappa_o)$. The spectral distribution of radiation is determined by finding a mean effective temperature and line of sight column density for the radiating molecules, computing intensity for each line in the band with the line function $L(\kappa_o)$, summing the line emission rates and scaling each line emission rate so that the total band intensity is obtained.

The use of band radiative transfer functions derived by assuming non-overlapping lines with Doppler shape does not lead to a completely satisfactory integration with the radiation field at lower altitudes. Gille and Ellingson (1968) have computed correction factors to make possible the inclusion of Doppler broadening effects in the computation of transmissivities of random exponential bands based on Lorentz line profiles. A rational approximation to their table of correction factors, obtained by a least squares gradient search on the parameters involved, has been investigated. Results were not good, partly because of the inaccuracy in computing transmissivity differences between

large values of absorber amount and partly because of the crudeness of the rational approximation, which in some cases led to differences with the wrong sign. Another problem with using such models is the difficulty of properly accounting for irradiation from an extended source (cf. Kuhn and London, 1969). Line-by-line integration with use of a Voigt line profile as done by Arnold, et al. (1969) is feasible when vibrational excitation is known beforehand and would be better but much slower than the present method of computing limb radiance spectral profiles.

Table III-1 lists the molecular bands included in the program. The band strengths listed for CO_2 , H_2O , O_3 and N_2O were adopted from a compilation by C. R. Calfee of ESSA which was provided by R. A. McClatchey (private communication, 1970) of AFCRL. These total band strengths agree with those obtained by summing the individual line strengths used by McClatchey, et al. (1970). The band strength of the fundamental of nitric oxide is an average of the values obtained by Abels and Shaw (1966), Feinberg and Camac (1967), Oppenheim, et al. (1967), Schurin and Clough (1963), and Varanasi and Penner (1967). The nitric oxide overtone value is that obtained by Schurin and Ellis (1966) and agrees with the theoretical calculation of Michels, et al. (1970).

D. Chemiluminescence

It is well known that some reactions such as that of atomic hydrogen with ozone to form OH lead to product molecules which are vibrationally excited and radiate in the infrared spectral region. Thus, Corbin, et al. (1969) assumed that nitric oxide produced by reaction R42 was produced with an average of one vibrational quantum. Hushfar, et. al. (1971) have determined the initial vibrational populations of nitric oxide in states higher than the first excited level. Their results indicate that at most one molecule in 50 is formed vibrationally excited to the second or higher vibrational level.

Table III-1
Molecular Band Strengths at 296K

<u>Molecule</u>	<u>Band Center</u> <u>Wavelength, μm</u>	<u>Vibrational</u> <u>Transition*</u>		<u>Band Strength</u> $\text{atm}^{-1}\text{cm}^{-2}$
		<u>Upper</u> <u>State</u>	<u>Lower</u> <u>State</u>	
CO_2	18.37	11102	10001	0.00675
	16.74	11102	02201	0.129
	16.18	10002	01100	3.56
	15.46	11102	10002	0.550
	14.98	01100	00000	205.0
	14.98	02200	01100	16.1
	14.97	03300	02200	0.948
	14.52	11101	10001	0.369
	13.87	10001	01100	4.59
	13.48	11101	02200	0.196
	12.64	11101	10002	0.0278
	10.41	00010	10001	0.0122
	9.40	00010	10002	0.0157
	5.18	11102	00000	0.0102
	4.82	11101	00000	0.0553
	4.26	00010	00000	2380.0
H_2O	6.27	010	000	290.0
O_3	9.60	001	000	320.0
	9.06	100	000	8.26
NO	5.33	1	0	112.0
	2.68	2	0	1.95
N_2O	17.26	0200	0110	1.73
	16.98	0110	0000	30.4
	16.98	0220	0110	1.73
	8.56	0200	0000	11.1
	7.78	1000	0000	216.0
	7.74	1110	0110	7.75
	4.58	0001	0000	1710.0

*Vibrational states are designated by ν , $\nu_1\nu_2\nu_3$, $\nu_1\nu_2\nu_3$, or $\nu_1\nu_2\nu_3$, where ν_i is the quantum number of the i th vibrational mode, ν is the vibrational angular momentum quantum number and f (if greater than zero) identifies different components of a Fermi resonance multiplet.

If their fit of the distribution to a relative vibrational temperature of 5000 K holds for the first vibrational level also, then this reaction will be of negligible importance in producing infrared radiation. No experimental data exists on the vibrational state of nitric oxide formed by the more important reaction of $N(^2D)$ with molecular oxygen, and nitric oxide chemiluminescence is not included in the radiance model. Similarly, F. R. Gilmore (private communication to J. W. Carpenter, 1970) has suggested that ozone may be formed in highly excited vibrational states which may lead to radiation occurring in the ν_3 mode at longer wavelengths than the 001 to 000 transition. Again, there has been no experimental determination and refinement. Gilmore's estimates would require more information on both the initial state of the product ozone molecule and the relative transition probabilities of the competing radiative transitions that cascade to the ground vibrational state.

SECTION IV

DESCRIPTION OF PROGRAMS

This section describes the computer programs developed to implement the chemistry discussed in Section II and the computation of high altitude limb viewing infrared radiances employing the physical processes discussed in Section III. The chemistry program, including the effects of vertical eddy mixing and molecular diffusion, is completely new. The programs to compute radiance are modifications of those developed by Corbin, et al. (1969). An additional program has been written to selectively plot the output of the radiance program. The programs are described below and are listed in the Appendix.

A. Chemistry Program

The chemistry program consists of a main program, SNAPS2, and 6 subroutines; ROMTST, TKEL, SOLLY, CONCEN, COLUMN, and SUNPHI. The main program performs the chemical computations, including the effects of vertical transport. ROMTST embodies the extrapolation method of Equation (2-18). TKEL is used to compute temperatures at each altitude. SOLLY computes the solar zenith angle and fraction of the solar disk visible at each altitude. COLUMN integrates the number densities of molecular nitrogen, oxygen and ozone above a given altitude in the direction of the sun. CONCEN is called by COLUMN to obtain number densities required for the integration. SUNPHI computes the attenuation of solar flux by absorption between a given altitude and the assumed top of the atmosphere in the solar direction and returns the photodissociation rates required for the chemistry.

The necessary input data to the chemistry program is a set of 14 data cards containing identification and variable parameters and a set of 603 cards containing concentrations of N_2 , O_2 , $O(^3P)$, O_3 , OH, H, H_2O , HO_2 , H_2O_2 , H_2 , CH_4 , CO_2 , CO, $O(^1D)$, $N(^4S)$, NO, NO_2 , N_2O , $N(^2D)$ and Ar at one km intervals between ground level and 200 km. The data is read in the following order:

1. IDENT 60 characters of identifying comments which are used in output page headings. The first character should be a blank.
2. DTHETA Co-latitude, degrees, of the computation location. A value of zero corresponds to the north pole.
3. DPHI East longitude, degrees, of computation location.
4. SOLDEC Solar declination angle, degrees, used to determine time of year.
5. GREF Surface gravitational acceleration, cm/sec^2 , at computation location.
6. REFF Effective value of earth radius, km, for use in computing gravitational accelerations at points above ground level.
7. EPS Relative error permitted for each time step in the integration.
8. MLMAX Maximum number of times integration is to be attempted for each time step to obtain relative error EPS.

9. **NBASE** Index of base altitude for computations, altitude in km plus one.
10. **NTOP** Index of highest altitude in computations, altitude in km plus one, restricted to 201 or less in current program.
11. **IHRMAX** Number of times at which complete output is required.
12. **MMAX** Number of integration steps between complete output points.
13. **DLTIME** Integration interval, seconds; the total simulated time for a given run, in seconds, is $IHRMAX*MMAX*DLTIME$.
14. **TIME** Initial time, seconds, measured from noon; A.M. values are negative, P.M. values are positive.
15. **CONSP** The 603 cards containing concentrations and identifying indices; concentrations are read into array CONSP.

Program execution begins with the initialization of constants used by the program. The values of eddy diffusion coefficients used at altitudes above 40 km are stored in array EDCOEF. The peak value set by the DATA statement occurs at 104 km. The eddy diffusion coefficient profile is lowered by 9 km in the DO loop ending with statement 90 and the low altitude eddy diffusion coefficients in array EDCF are transferred to array EDCDEF in the DO loop ending with statement 95. This permits use of separate sets of high and low altitude diffusion coefficients by changing the appropriate data

statements, and easy variation of the altitude of maximum turbulent transport. The data described above is then read in. The information on each data card is written to printer output channel 6 as it is read. Columns 13 through 80 of the second through fourteen data cards are printed in addition to the number placed in columns 2 through 12 so that comments may be added. The first 14 data cards are printed on a page numbered -1. The input concentrations require about 10 pages to print, the first of which is numbered page 0. Further execution is determined by the input data. A brief flow chart is given on the following pages.

The outermost control DO loop ending with statement 450 is executed IHRMAX times. Within this loop, the computer clock is called and computer running time since the beginning of the program is stored in variable SECA. Variable locations used in the DO loop ending with statement 110 are set to zero and this loop is entered and executed for each altitude between NBASE and NTOP. The mean molecular mass RMWT at each altitude is computed by the statements associated with DO loop 102. Temperatures are computed by calls to function TKEL. The gravitational acceleration at each altitude is computed and local mixing scale heights H_{av} are computed. Coefficients for the eddy diffusion contributions to q and β terms in Equation (2-10) are determined from the finite difference approximation, Equation (2-8), and stored in arrays BTED, QJEDL and QJEDU. Factors needed for computation of molecular diffusion contributions are computed and stored in arrays AFAC, BFAC, CFAC, DFAC and RDTEMP. The molecular concentrations at each altitude above the base altitude are scaled to be consistent with the finite difference scheme in the DO loop ending with statement 104. An effective molecular scale temperature is used for the local scale height. Before exit from DO loop 110, N_2 and O_2 concentrations and sample computed values are written to the printer output channel for altitudes between but not including those associated with NBASE and NTOP.

Flow Chart for Chemistry Program

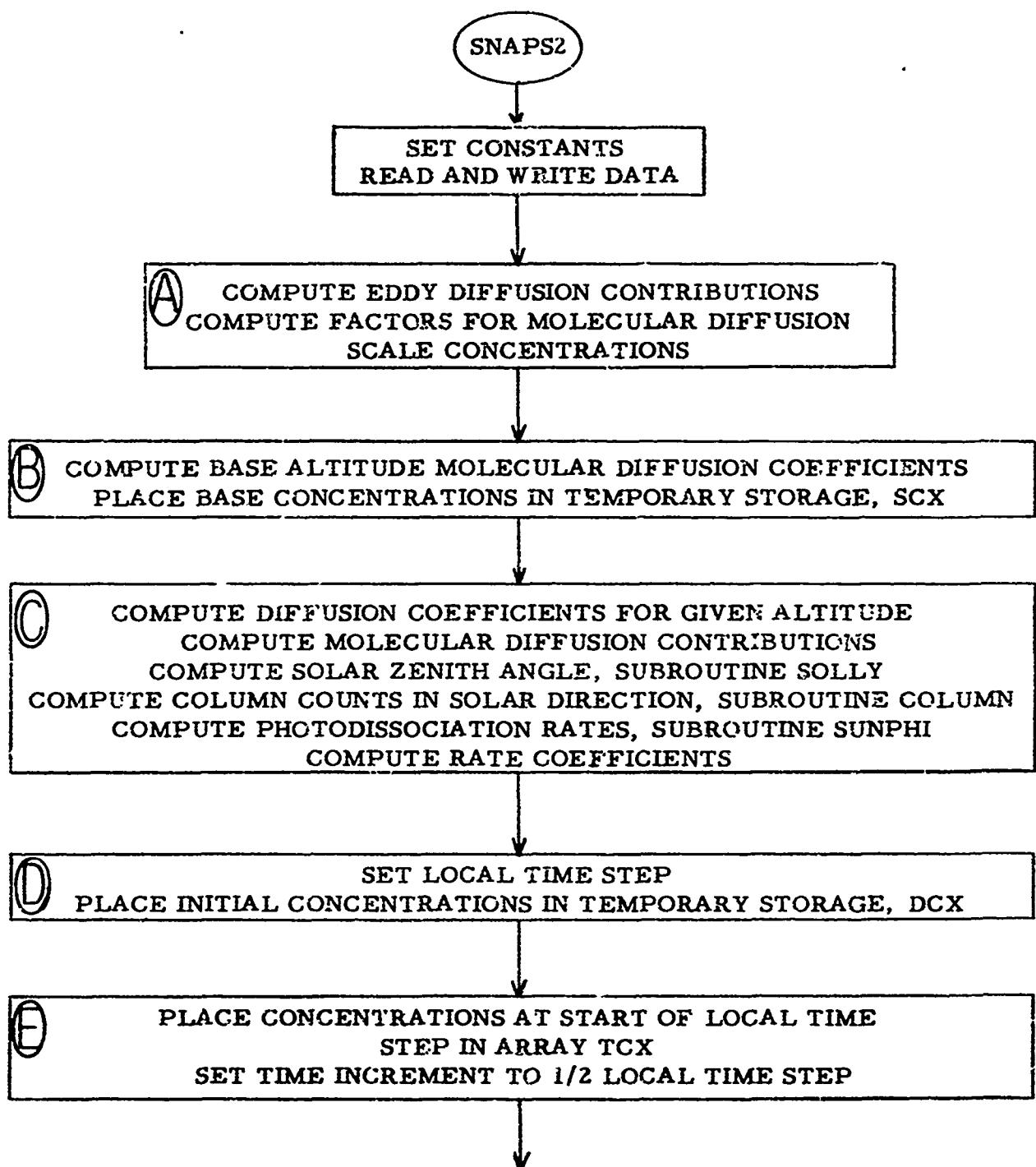
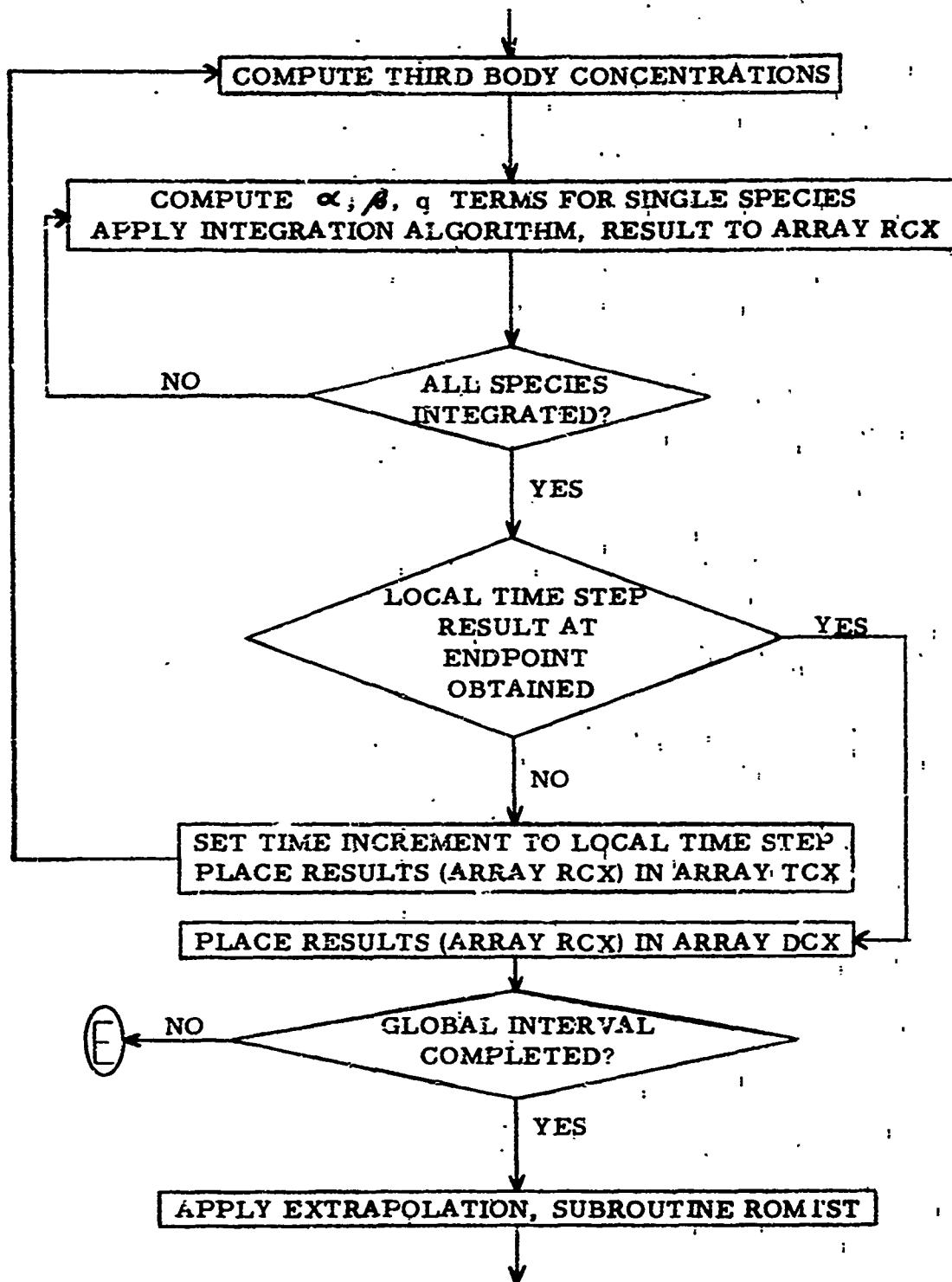
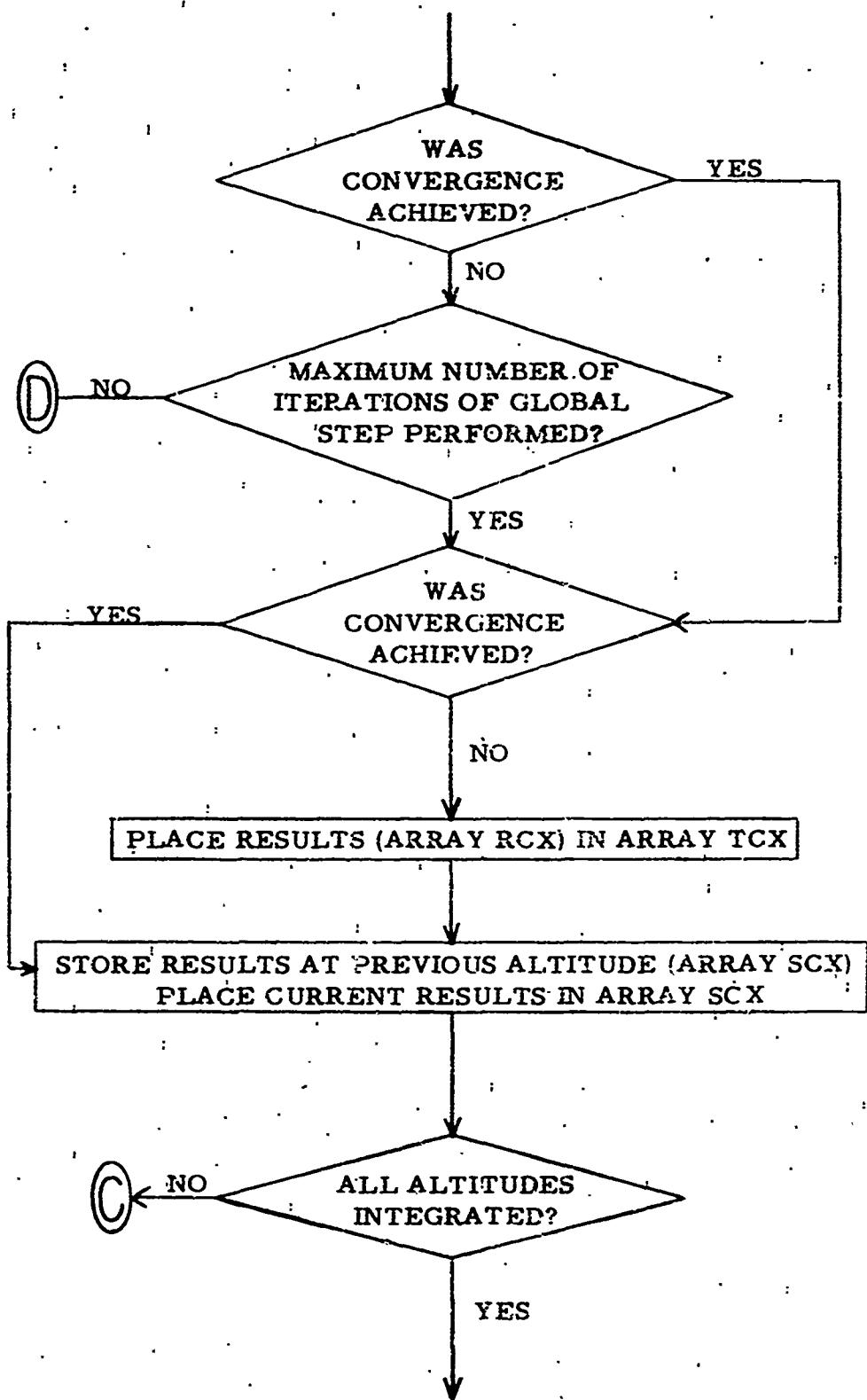


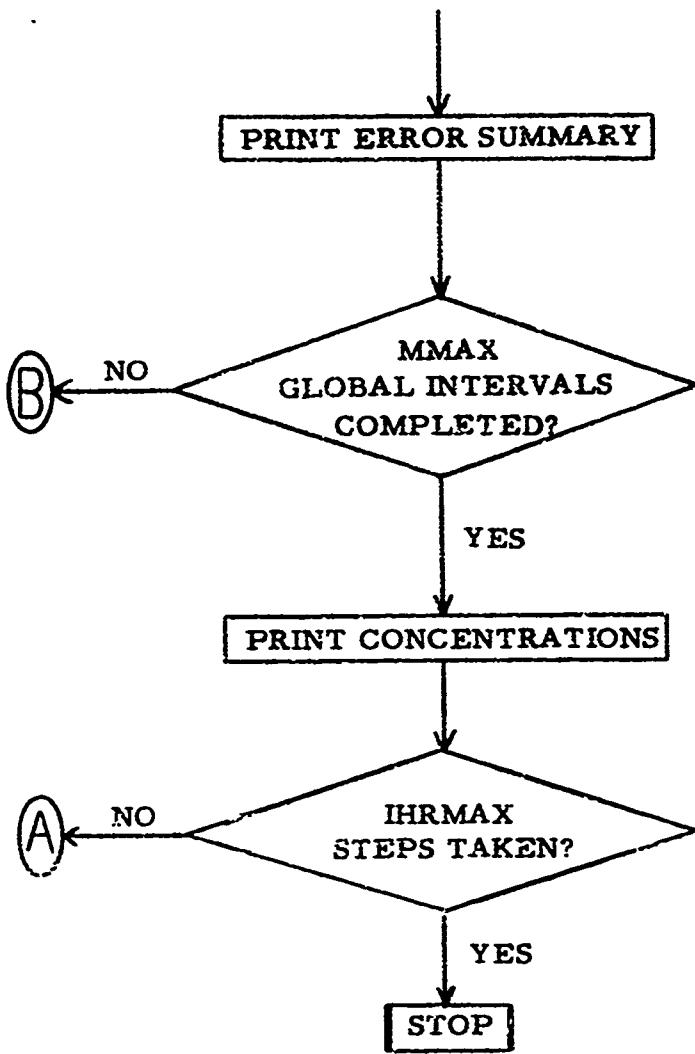
FIG. Chart for Chemistry Program (continued)



Flow Chart for Chemistry Program (continued)



Flow Chart for Chemistry Program (continued)



The DO loop ending with statement 400 is entered and executed MMAX times. Each execution advances the integration time by DLTIME seconds. The time at the end of the step is computed in floating and fixed point form. If the value of NPRNT permits, a new page is started and the time and column headings are printed. Molecular diffusion coefficients are computed for the two lowest altitudes in the statements associated with DO loop 130.

The DO loop ending with statement 350 is entered and executed for each altitude. Molecular diffusion coefficients are computed for the next higher altitude, and the molecular diffusion contributions to the β and q terms are computed and combined with the eddy diffusion contributions in the DO loop ending with statement 140. The solar zenith angle CHI and the fraction ETA of the sun's disc visible are computed by subroutine SOLLY. If the sun is visible, column counts of N_2 , C_2 , O and O_3 in the solar direction are computed in subroutine COLUMN and photodissociation rates are computed in subroutine SUNPHI for the time at the midpoint of the time interval of integration. Reaction rate coefficients are computed for the temperature at the given altitude.

The integration for a global time increment DLTIME at a single altitude is performed in the DO loop ending with statement 300. The operations within this loop are repeated either until convergence to relative accuracy EPS is achieved or until MLMAX repetitions have been performed with no convergence. Each time through this loop, a new number of local time intervals, MMF, is computed to conform to the extrapolation procedure of subroutine ROMTST. Values of the initial concentrations at the integration altitude in array CONSP are placed in array DCX. The DO loop ending with statement 290 then integrates over the MMF local time steps. The values in array DCX are copied into array TCX and the time increment DTIME is set to one-half the length of the local increment. An index ITER is set to one and appropriate third body concentrations

are computed. The algorithm of Equation (2-10) is then applied for each species in the DO loop ending with statement 255, the results being placed in array RCX. ITER is incremented and the results in array RCX are placed in array TCX. The time increment is doubled and the DO loop ending with statement 255 is again executed, using the intermediate results from the first execution to compute the α , β and q terms. The results of this second cycle, computed in array RCX, are transferred to array DCX and the statements in the DO loop ending with statement 290 repeated until the global time interval DLTIME has been covered. Subroutine ROMTST is called to test the values in array DCX with previous results produced in the DO range ending with statement 290. The improved concentration values are returned in array TCX. If convergence is achieved, control is transferred to statement 310. Otherwise, the DO loop ending with statement 300 is repeated. If this process does not result in convergence in MLMAX tries, the endpoint values in array RCX are placed in array TCX in the DO loop ending with statement 315. The endpoint results for the next lower altitude, which have been stored in array SCX, are written into array CONSP and the contents of array TCX are placed in array SCX. Production rates for OH by two different reactions are computed and stored in QCOHA and QCOHB. "Rectangular" sums of total column counts are incremented in DZOHA and DZOHB. These values are computed to provide a rough check on the hydrogen compound chemistry and may be compared with airglow observations. If the value of NPRNT permits, the altitude, QCOHA, QCOHB, DZOHA, DZOHB and the concentrations of 16 molecules are written to the printer output channel. The statements in the DO loop ending with statement 350 are then repeated until concentrations at all altitudes between (but not including) NBASE and NTOP have been integrated over the global time step DLTIME.

When all altitudes have been integrated, a summary of number of iterations is sent to the printer output channel and the time value TIME is

incremented by DLTIME.

After the integration has been advanced MMAX times with the increment DLTIME, all concentrations are sent to the punch output channel by the statements in DO loop 420 and to the printer channel by the statements in DO loop 440. The internal computer clock is again accessed and the starting, end, and elapsed time required in DO loop 450 are sent to the printer output channel. Program execution ceases after this outer DO loop has been executed IHRMAX times.

The scaling of concentrations performed in the DO loop ending with statement 104 permits use of output data from runs at another latitude or with a different temperature profile to be used as input data. While there may be some difficulty in reaching convergence at altitudes below 90 km in the first time step, this is not a serious problem. When using a global time step DLTIME of 600 seconds and a value of 0.01 for EPS, computation of chemical changes over a day for 150 altitudes requires on the order of 20 minutes running time on the CDC 6600. This is longer than would be required by the differencing methods usually employed (e.g., Shimazaka and Laird, 1970) but the error control compensates for this. It is not necessary to alter time increments at dawn or sunset since the convergence algorithm of subroutine ROMTST automatically forces the use of smaller time subdivisions of the global time interval DLTIME. Further study is required before it will be possible to state optimum values of DLTIME and MLMAX. Since as many as 20 diurnal cycles may be required to reach concentrations which repeat from one simulated day to the next, a means of reducing running time is required. Possible methods are to rewrite the program and subroutines COLUMN, CONCEN and TKEL to use a larger altitude increment or to generate a starting atmosphere with the method of Colegrave, et al (1966). In its present form, the chemistry program SNAPS2 uses fixed concentrations of NO^+ , O_2^+ , O^+ and electrons during the day and assumes no ions to be present at night. The full ionic chemistry of Table 2-4 should be added and photoionization rates added to the photodissociation

rates computed by subroutine SUNPHI.

The names of the real arrays and their uses are:

AFAC	stores values of numerical approximation to $\frac{1}{T} \frac{\partial T}{\partial z}$
AMWT	stores values of molecular weights, gm/mole; values are set by data statement
BFAC	stores values of the coefficient of molecular concentration in the numerical approximation to $-\left[\frac{\partial^2 n}{\partial z^2} + \frac{1}{T} \frac{\partial^2 T}{\partial z^2} n - \frac{1}{T^2} \left(\frac{\partial T}{\partial z} \right)^2 \right]$
BTED	stores values of coefficients used in computing contribution to β terms from eddy diffusion
BTEMD	stores values of contribution to β term from both eddy and molecular diffusion for each molecule at a given altitude during integration.
CARD	used as temporary storage for comments in columns 13 through 80 of first 14 data cards
CFAC	stores values of numerical approximation used to compute $\frac{1}{H^2} \frac{\partial H}{\partial z}$ for diffusive scale heights
CMD	stores values of molecular diffusion coefficients for each molecular species at a given altitude during integration
CMDL	stores values of CMD at next lower altitude
CMDU	stores values of CMD at next higher altitude

COL	stores values of integrated column counts computed by subroutine COLUMN
CONSP	stores values of molecular number densities; initial values are read in from cards; values are altered at each integration step
DCX	stores initial number densities for one altitude during local time step in integration
DFAC	stores values of g/RT used in computing atmospheric scale heights and contribution of molecular diffusion
EDCF	stores values of eddy diffusion coefficients for altitudes below 40 km, set by DATA statement
EDCOEF	stores values of eddy diffusion coefficients, initially contains high altitude values set by DATA statement
QJEDL	stores coefficients of eddy diffusion contribution to q terms from next lower altitude
QJEDU	stores coefficients of eddy diffusion contributions to q terms from next higher altitude
QJEMD	stores values of contribution to q term from eddy and molecular diffusion for each molecular species at a given altitude during integration
RATE	stores values of photodissociation rates computed by subroutine SUNPHI
RCX	stores intermediate values of number densities for a single altitude computed during local time step in integration

RDTEMP	stores values of temperature coefficients used in computing molecular diffusion coefficients
SCX	stores values of number densities computed at end of global time step for next lower altitude; values eventually replace corresponding numbers in CONSP
TCX	stores intermediate values of number densities used in computing α , β and q values during integration of local time step for a single altitude
TEMPK	stores values of temperatures at each altitude, values are computed by function TKE L
TETOT	stores values of total electron densities at each altitude, values are set by DATA statement
TFMT	stores format statement for computer running time printout, set by DATA statement
TINO	stores values of NO^+ concentrations at each altitude, set by DATA statement
TIO	stores values of O^+ concentrations at each altitude, set by DATA statement
TIO2	stores values of O_2^+ concentrations at each altitude, set by DATA statement
TST	used as workspace by subroutine ROMTST

The names of integer arrays and their uses are:

IDENT	stores 60 character comment read from first data card, which is used in page headings
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IDNT	stores image of last 20 characters of first data card
LSP	stores hollerith constants used in printing column headings
MLPRNT	stores data on number of iterations required for convergence of integration at a given altitude, and (largest) index of species which did not converge in MLMAX iterations

The names of the real variables and their uses are:

AFACNA	temporary storage of value of AFAC for altitude at which integration is being performed
BFACNA	temporary storage of value of BFAC for altitude at which integration is being performed
BTEDNA	temporary storage of value of BTED for altitude at which integration is being performed
BTSQ	square of β term used in integration
BTT	value (partial or complete) of β term used in integration for a single molecular species
CFACNA	temporary storage of value of CFAC for altitude at which integration is being performed
CHI	solar zenith angle, radians, computed by subroutine SOLLY
CHISAV	temporary storage for value of CHI
CMDSNP	temporary storage for value of molecular diffusion coefficient for single molecular species

CON	temporary storage for factor used in scaling molecular concentrations at altitude NTOP to fit scale height defined by molecular scale temperature
CONFAC	temporary storage for factor used to scale molecular concentrations to fit local scale heights defined by molecular scale temperature
CONSPN	temporary storage for concentration of a single molecular species at a given altitude
C1	temporary storage for molecular nitrogen concentration
C2	temporary storage for molecular oxygen concentration
C3	temporary storage for atomic oxygen concentration
DCT	temporary storage for single value from array DCX
DDDZ	temporary storage for value of $\frac{\partial D}{\partial z}$ for single molecular species
DELZ	altitude increment, cm
DFACNA	temporary storage for value of DFAC at altitude for which integration is being performed
DHDZ	temporary storage for value of $\frac{\partial H}{\partial z}$
DKDZ	temporary storage for value of $\frac{\partial K}{\partial z}$
DLT	value of δ used in integration for a single molecular species

DLTIME	time increment for integration step, read in as data
DPHI	east longitude of point of integration, read in as data; not needed in present program which assumes times are true solar times
DTDZ	temporary storage for value of $\frac{\partial T}{\partial z}$
DTHETA	colatitude of point at which integration is performed, read in as data
DTIME	storage for value of local time step in integration
DZOHA	values of integrated production rates of OH
DZOHB	
ED	temporary storage for value of eddy diffusion coefficient at a given altitude
EPS	value of relative error allowed in integration
ETA	fraction of solar disc visible at given altitude
FAC	temporary storage for intermediate results, use varies in different parts of program
FACB	temporary storage for either βt or δt in Equations (2-10)
FACDMB	temporary storage for $\delta - \beta$ in Equation (2-10a)
FACM	temporary storage for value of $1 - \exp(-\delta t)$
FACRT	temporary storage for $4\alpha q/\beta^2$
FAC2AX	temporary storage for $2\alpha x_0$
FAC4AQ	temporary storage for $4\alpha q$

G	value of gravitational acceleration at altitude NALT
GL	value of gravitational acceleration at altitude NALT - 1
GREF	surface value of gravitational acceleration, read in as data
GU	value of gravitational acceleration at altitude NALT + i
QCOHA	values of OH production rates at altitude of integration
QCOHB	
QJEDLN	temporary storage for value of QJEDL at altitude of integration
QJEDUN	temporary storage for value of QJEDU at altitude of integration
QJT	temporary storage for partial or complete value of q term used in integration of a single molecular species
RDELZ	reciprocal of twice the altitude increment DELZ
RE	effective radius of earth, km, used in geometrical computations
REFF	effective radius of earth, km, used in gravitational calculations, read in as data
RFAC	temporary storage of intermediate results
RII....	storage for values of ionic reaction rates
RMWT	mean molecular mass at altitude NALT

RMWTL	mean molecular mass at altitude NALT - 1
RMWTU	mean molecular mass at altitude NALT + 1
ROBS	altitude of given point, km
RTIME	variable used in printing time values
R1, ...	values of forward neutral reaction rates
R2DELZ	square of reciprocal of altitude increment, DELZ
SECA	storage for value of computation of computer running time
SECB	
SECC	
SFAC	temporary storage of intermediate results
SH	value of mixing scale height at altitude NALT
SHL	value of mixing scale height at altitude NALT - 1
SHU	value of mixing scale height at altitude NALT + 1
S11, ...	values of reverse ionic reaction rates
SOLDEC	solar declination angle, read in as data
SUM	temporary storage used in forming mean molecular masses
SUML	
SUMU	
S1, ...	values of reverse neutral reaction rate coefficients
TCH4, ...	values of individual molecular concentrations in array TCX, names individually for convenience in forming α , β and q coefficients: TCH4 corresponds to CH_4 , TCO corresponds to CO, etc.

TEMP	value of temperature at altitude NALT
TEMPI	reciprocal of temperature
TEMPL	value of temperature at altitude NALT - 1
TEMPU	value of temperature at altitude NALT + 1
TEMP12	value of minus one-half power of temperature
TEMP32	value of minus three-halves power of temperature
TEMP52	value of minus five-halves power of temperature
TFAC	temporary storage of intermediate results
TIME	time, expressed in seconds from noon, read in as data; altered in program to be the time at midpoint of a global integration step so that approximate mean values of photodissociation rates will be computed by subroutine SUNPHI
XM4, . . .	third body concentrations for appropriate three-body reactions
XXX12	storage for factor used in computing q term for CO_2 and β term for CO

The names of integer variables and their uses are:

I	index in DO loop 95, auxiliary index in DO loop 110, and index in implied input/output DO loops
IF	final parameter in innermost implied DO loop used in printing output concentrations within DO loop 440

IHR index in DO loop 450

IHRMAX final parameter in DO loop 450, input as data

IP index in print control DO loop 440

IS initial parameter in implied DO loop, see IF

ITER control index in integration, used between statements 200 and 260 to select proper values for array TCX

IX index in DO loop 435, incremented for each page of output

J index in implied DO loops used in reading data into array CONSP within DO loop 100

KCH4, ... index variables used to select appropriate values of quantities related to given species; most uses replaced by use of TCH4, etc.

KTEST parameter returned by subroutine ROMTST, zero if integration has converged, non-zero otherwise

LALT, LCHI,
LCOLN2,
LCOLO2,
LCOLO3,
LDZOHA,
LDZOHB,
LJO2, LJO3,
LML, LQCOHA,
LQCOHB,
LTIME store Hollerith constants used in printing column headings and are set by DATA statements

M	index of DO loop 400, incremented for each global time step
ML	index of DO loop 300, incremented for each iteration of integration over global time step at a given altitude
MLMAX	final parameter of DO loop 300, read in as data
MLSAVE	temporary storage for value of ML, used after exit from DO loop 300 to print number of iterations required for convergence
MMAX	final parameter of DO loop 400, read in as data
MMF	final parameter of DO loop 290, computed from ML and is number of local subdivisions of global time step DLTIME for the MLth iteration of integration
MMS	index for DO loop 290, see MMF
NA	auxiliary index, usually set to NALT - 1
NALT	index for DO loops 90, 100, 110, 350, 420 and 430; denotes a given altitude
NAMIN	value of NALT - 1 in DO loop 350
NB	value of NALT - 2 in DO loop 110
NBASE	index of lowest altitude for integration, read in as data
NF	final parameter of DO loop 430
NMIN	stores input value of NBASE, which is changed by program

NPAGE	stores output page number
NPLU	value of NALT + 1 in DO loop 350
NPRNT	variable available to control output of concentrations at integration steps intermediate to fully documented output at end of DO loop 450, set to 1 at present, so values are output for each interval DLTIME
NS	initial parameter of DO loop 430
NSP	index in DO loops 102, 104, 130, 140, 180, 190, 255, 258, 280, 315, and 320; a value of NSP selects a value of a variable corresponding to a single molecular species
NSPM	number of molecular species included in program, 20 at present, used as final parameter of DO loops with NSP as index
NT	final parameter of DO loop 420, in which output cards are punched
NTIME	used in printing time values
NTOP	index of highest altitude used in integration, input as data
NW	channel number for printing computer running time information, set to 6 here
NXX	temporary storage for altitude index read from cards containing concentration data
N1	storage space used for sequence numbers of cards read in or punched out at a given altitude
N2	
N3	

B. Radiance Program

The high altitude radiance programs of Corbin, et al. (1969), BCKGND and SPCTRA, have been modified by the addition of six carbon dioxide

bands between 5 and 25 μm , and improved band modeling for the water vapor 6.3 μm band and the ozone 9.1 and 9.6 μm bands. The basic structure is unaltered and the division into two programs is retained. The organization of the CDC 6600 program control system makes this feasible and the overall saving in central memory storage space is greater than would be possible by using overlays. The output from the three lower altitude programs of Corbin, et al (1969), which are based on Anding's (1968) program, is required only to produce values of vertically directed radiances at the band centers. The programs INTERP and CATM were run to produce on cards a complete set of input data to RAD for each of the 47 lower atmosphere models. RAD was modified slightly to permit reading in the band data cards and to either write on tape or punch the band data cards with appropriate values of upwelling flux, TFLUX. The mid-latitude winter atmosphere model was used for the present computations.

Program BCKGND consists of the main program BCKGND and subroutines BANRAD, INTERP, SIMP, XFER, TAUMAX, SJMAX, SDM2, SM1, SLM1, QJPART, and EVAL. Program SPCTRA contains the main program SPCTRA and subroutines ROTATE, SFUN, QINT, FILTER, WATSTR, ROTSTR, ROTPOS, and SIMP. Overall operation is discussed below.

The main program BCKGND serves primarily to control the operation of subroutines which compute vibrational populations and radiative rates. BCKGND reads and checks the input data, and transfers control to subroutine BANRAD which computes vibrational populations, local optical thicknesses and volume radiances for all included bands of a single molecular species. When control is returned, BCKGND computes and outputs integrated band radiances for limb viewing (exoatmospheric) and seven endoatmospheric viewing angles at selected tangent heights or endoatmospheric altitudes.

Data is read in on two different channels, one being used for number densities and collisional excitation rates, the other for band data which is needed again by program SPCTRA. The storage space used for methane data in the older version is now used for atomic oxygen concentrations. After input

data is checked, control is transferred to subroutine BANRAD.

BANRAD computes the population of vibrational levels of infrared active species, including the effects of collisional excitation; absorption of radiation from the lower atmosphere, sun and molecules radiating at high altitude. The values returned to the main program are volume radiance and unit optical thickness at each altitude for each band included in the computation.

The first step in the computation is determination of the thermal equilibrium populations of vibrational levels. This is performed in the DO range ending with statement 130. Each passage through this DO range computes populations for one altitude. Within this DO range are two others. The DO range ending with statement 110 computes the vibrational population of each level relative to the ground vibrational level, using the energies (wavenumber) stored in WAVE and the statistical weights stored in the ten's places in LSC. The relative populations are stored temporarily in real array VIEPOP. The sum of relative populations is stored in SUM. The final ground state population is then computed by dividing total concentration by SUM, and stored in real array GNDSTE. The DO range ending with statement 120 then computes the vibrational population of each level by multiplying total concentration by relative configuration divided by SUM.

The DO range ending with statement 135 selects the vibrational level which is coupled with the first excited nitrogen vibrational level.

The DO range ending with statement 160 computes the rate at which a single molecule in a given level is excited or de-excited by collisions at each altitude.

The outer DO range ending with statement 180 computes wavelengths (BNDLAM), Einstein A coefficients (EA), G factors for absorption of radiation from the sun (GDOWN) and from the earth and lower atmosphere (GUP) and the

G factor used in computing radiative transfer within the upper atmosphere (GFAC). The inner DO range ending with statement 180 computes the unit optical thicknesses for each band at each altitude using function TAUMAX, and stores the result in array BNDTAU. In addition, it computes the volume radiances and stores them in array BNDRAD. Further computation is then performed iteratively in the DO range ending with statement 400.

The DO range ending with statement 190 computes various integrated optical thicknesses for each band. The DO range ending with statement 182 computes the total optical thickness between each two altitudes in the vertical direction and stores the values in array TTH. The DO range ending with statement 184 (1) computes the total optical thickness between the base altitude and each other altitude, storing the result in array TTIP and (2) computes the total optical thickness between the top altitude and each other altitude, storing the results in array TTDOWN. If the computation is not for daytime conditions, the DO range ending with statement 186 sets the values in TTDOWN equal to 0.0, for efficiency in the later computations.

Computation of vibrational populations is done separately for each species. Control is transferred to statement 220 for CO_2 , statement 230 for H_2O , statement 240 for NO, statement 250 for N_2O or statement 230 for O_3 . The DO range following each of these statements is used to compute vibrational populations. After each set of vibrational populations is completed, new values of volume band radiances are computed in the nested DO ranges ending with statement 360. Following three iterations, vibrational populations are written to an output file for use by program SPCTRA and control is returned to the main program.

BANRAD returns volume emission radianc values in array RAD and local optical thickness values in array TAU. For each band, line of sight band radiances are computed in the DO range ending with statement 840. Then

trapezoidal rule integration is performed to determine the radiance arising along each of the eight lines of sight, including the modification necessary for the effects of optical thickness along the line of sight. The DO range ending with statement 830 controls the integration for each tangent height and endo-atmospheric viewing level. Radiance values are computed at 5 km intervals of tangent height up to 150 km and at 25 km intervals above this level. The integration of radiance values is performed for each endoatmospheric viewing level in the DO range ending with statement 810. The integration begins at the viewing altitude. At each point on the line of sight, the contribution of the local volume emission rate to that received at the viewing point is computed by subroutine SMI which takes into account the effects of optical thickness between the emitting point and the viewing point. The equivalent integration for the limb viewing case is performed in the DO ranges ending with statements 815 and 818. Upon completion of the integration for each tangent height and endoatmospheric viewing level, band radiances for that level are both printed and written to the output file used by BANRAD, for input to SPCTRA.

Program SPCTRA computes the spectral radiances between 5 and $25 \mu\text{m}$ corresponding to the band radiances computed by BCKGND. The input data to SPCTRA are the molecular vibrational level and band data also used by BCKGND, the vibrational population and band radiance data generated by BCKGND, and individual line data for the water vapor rotational lines and ν_3 band and the ozone ν_3 and ν_1 bands. The later data was obtained from R. A. McClatchey through the contract monitor.

When program execution begins, values are assigned to the integer variables NOUT, NLN and NALT and the subroutine ROTATE, which reads in data for the individual lines, is called. The outer DO range ending with statement 500 is entered. The DO parameters are fixed at present to produce two sets of spectra, using night and day input from program BCKGND. The program may be

made more flexible by reading in DO parameters prior to execution of the DO statement. The variable BLAM is set to 5.0 and the outer DO range ending with statement 105 is entered. The effect of the first two statements is to set up a table of wavelengths at $0.1 \mu\text{m}$ intervals between 5 and $25 \mu\text{m}$ in real array AVLAM. These are the wavelengths at which spectral radiances are printed out. Again, more flexibility may be achieved by making the intervals and spacing dependent on values read in. If this is done, corresponding changes must be made in subroutine FILTER. The inner DO range ending with statement 105 sets the values of output spectral radiances equal to zero. Temperatures are set in the DO range ending with statement 110.

Next, the number of molecular species is read in and stored in integer variable NSPTOT. The outer DO range ending with statement 400 is entered and executed NSPTOT times. Within this DO range, molecular vibrational level and band data and vibrational population data are read in and mean temperatures and total number of molecules per unit area in the vertical and horizontal directions are computed for each vibrational state. Total band radiances corresponding to limb viewing and vertical and horizontal endoatmospheric viewing are read in. Relative line radiances are computed and normalized to the total band radiances. The spectra corresponding to the normalized line radiances are computed and stored in arrays SPECA, SPECB and SPECC. Details of these computations are given below.

The code number of the species ISP is read in. The number of vibrational levels NLEVEL, the number of bands NBAND and the molecular weight RM are read in. In the DO range ending with statement 210, the level description codes LSC and LCC, the energy and the mean rotational constant for each vibrational level are read in. In the DO range ending with statement 220 the band description codes LBC and LBU and the band strength for each band are read in. The number of altitudes NALT for which vibrational populations are computed for the species

and the number of altitudes NRLEV for which band radiances are computed by BCKGND are read in. Vibrational level populations are read in and stored in array CON.

The mean temperatures and total number of molecules per square centimeter in the vertical and horizontal directions at 5 km intervals between 60 and 115 km are determined in the DO range ending with statement 129. The product of temperature and vibrational level population is computed in the DO range ending with statement 112. The integrals of total number of molecules and the product of temperature and number density in the vertical direction are computed in the DO range ending with statement 120. Simpson's rule integration is used. The total number of molecules in a given vibrational level above a given altitude is stored in array COLCNT. The corresponding mean temperatures, obtained by dividing the integral of the product of temperature and number density by the integral of number density, are stored in array AVTEMP. After exit from DO range, the column counts and temperatures are printed out.

The DO range ending with statement 128 performs a similar computation for column counts and mean temperatures in the horizontal direction. The integrations required are performed in function QINT. Upon exit from this DO range, column counts stored in array HORCNT and mean temperatures stored in array BVTEMP are printed out.

The inner DO range ending with statement 400 is now entered and executed for each band. This DO range controls the computation of the spectra.

The altitude HT, the limb band radiance RADC, and endoatmospheric radiances RADA (upward direction) and RADB (horizontal direction) are read in the DO range ending with statement 230. Band information is computed from band and level constants. A test is made on the species code ISP to determine whether the molecule is linear or nonlinear.

Following the test of ISP, if the molecule is linear, line positions are computed in subroutine ROTPOS. The DO range ending with statement 250 is entered and executed for each of the twelve altitudes for which spectra are computed. Line radiances are computed in subroutine ROTSTR for vertical endoatmospheric viewing. Successive calls to subroutine FILTER compute the spectral contributions from lines in the P, Q, and R branches. The sequence of calls to ROTSTR and FILTER is repeated for endoatmospheric viewing in the horizontal direction and for limb viewing. Upon exit from this DO range, control is transferred to statement 280.

If the test on ISP determines that the molecule is non-linear (water vapor or ozone) control is transferred to statement 260 and the DO range ending with statement 270 is executed for each of the altitudes for which spectra are computed. For water vapor, spectra are generated from the pure rotational line radiances by calls to subroutine WATSTR and FILTER and for the 6.3 μm band by calls to WATSTR and FILTER, for each of the three viewing conditions. For ozone, spectra in the 9.1 and 9.6 μm bands are also generated by calls to WATSTR and FILTER.

Following the final execution of the DO ranges ending with statement 400, the spectra are printed out in the order endoatmospheric viewing in the upward direction, endoatmospheric viewing in the horizontal direction and limb viewing. Each of these sets is printed on four pages, successive pages covering 5-10 μm , 10-15 μm , 15-20 μm and 20-25 μm . The first column on each page contains wavelengths and successive columns contain radiance values at altitudes or tangent heights 60, 65, 70, ... km. The data in arrays AVLAM, SPECA, SPECB and SPECC are written to a binary file, either for immediate use by the plotting program or for transfer to magnetic tape for later use.

C. Plotting Program

The plotting program, TRYCRT, is designed to read the binary output tape produced by the spectral radiance program, SPCTRA. It consists of the main program, TRYCRT, and six subroutines, LINSCA, LOGSCA, LINAXS, LOGAXS, GRID and NULINE. In addition, it uses the AFCRL/CDC 6600 system subroutines which are needed to produce microfilm plots. The version listed in the Appendix is set up to plot three sets of radiances, assuming that the SPCTRA output tape contains two sets of data, with vertical and horizontal endoatmospheric radiances and limb radiance data in each set. This program further assumes that there are 12 different altitude profiles in each data set. Graphic output is written on tape 39 and microfilm is produced from this. The microfilm must then be reproduced on paper.

The program places the date of the run in the first word of array IDENT, which is plotted with each graph. The other 2 words of the array contain the user name and project number, stored by a data statement. The x-axis length, SX, is set to 9 inches and the y-axis length, SY, is set to 14 inches. The CDC 6600 subroutines are initialized by calls to subroutines CRTPLT and PLOT. The number of graphs to be plotted, NCASES, number of characters, NXL, in x-axis caption, XBCD, number of characters, NYL, in y-axis caption, and y-axis caption, YBCD, are read in from cards and printed on the line printer. The DO loop ending with statement 400 is then executed for each graph to be produced. Minimum wavelength, WVMIN, and maximum wavelength, WVMAX, are read. Plotting constants INF, NX and NY are computed. Wavelengths are read from the SPCTRA output tape (channel 2) and stored in array AVLAM. An appropriate subset is then stored in array X. These are then scaled by subroutine LINSCA. Radiance data are then read from channel 2 and stored in array SPCTRA. An appropriate subset is selected and stored in array Y. Values in Y are scaled for plotting by a call to subroutine LOGSCA. Line intensity is set to 16 by a call to subroutine STBEAM. Axes are drawn on all

four sides of the graph by calls to subroutines LINAXS and LOGAXS. Calls to subroutine GRID place vertical and horizontal grid lines on the graph. Radiance values are further scaled in the DO loop ending with statement 150. Radiance values are placed on the graph by calls to subroutine NULINE in the loop ending with statement 200. Line intensities for each curve produced in this loop are set by calls to STBEAM and use values stored in array JBEAM through a data statement. After each set of curves on a graph is produced, a call to subroutine FRAME prepares for a new graph. The DO loop ending with statement 250 is repeated three times, the first and second cycles plotting vertical and horizontal endoatmospheric radiances while the third plots limb viewing radiances. When only limb viewing radiances are desired, statement 250 should be placed immediately after the statement "read (2) SPCTRA" on line TCRT 540.

Subroutines LINSCA and LOGSCA were written to provide automatic scaling of data points in a manner which would utilize maximum space on the graph. In addition to scaling data points, these subroutines generate values KONX, DX, MINY and MAXY which provide data which is used in the axis drawing subroutines LINAXS and LOGAXS and the grid drawing subroutine GRID. The subroutine NULINE was written to replace the standard AFCRL/CDC 6600 subroutine LINE which draws straight lines between plots. NULINE permits points to be plotted a limited distance outside the graph boundaries if the data for a graph covers more than 9 orders of magnitude.

SECTION V

RESULTS AND DISCUSSION

Representative limb viewing radiance profiles are shown in Figures V-1 through V-5. These profiles result from the use of the nitric oxide, water vapor, ozone and carbon dioxide concentrations of Figures II-1 to II-4 and an assumed nitrous oxide volume mixing ratio of 5×10^{-7} in the upper stratosphere (Keneshea 1967). The model atmosphere for the computations, used primarily for the temperature and total density profiles, is taken from the U. S. Standard Atmosphere Supplements, 1966 and uses the 30° latitude January model below 120 km and the Spring/Fall model with exospheric temperature 1000 K above 120 km.

The results shown are not qualitatively different from those of Corbin, et al. (1969). The quantitative differences result primarily from the use of different molecular abundances. The use of a lower exospheric temperature has negligible effect because at the higher altitudes where the temperature is lower, the radiation is determined by absorption of radiation from the lower atmosphere or the sun and temperature dependent collisional processes play a negligible role. The nitric oxide fundamental band at 5.3 μm is an exception, because of the excitation by collisions with atomic oxygen. Even for this molecule, results are not appreciably different during the day. At night, however, limb radiances at 5.3 μm do not fall off as rapidly with altitude below 200 km. The carbon dioxide bands added do not make an appreciable difference in the limb radiances because the basic excitation mechanism for these bands is absorption of solar or terrestrial radiation in the weak combination and overtone bands at 5.18 and 4.82 μm .

Limb Viewing Spectral Radiances, 5 to 8.5 μm
Solid Line Day, Dashed Line Night

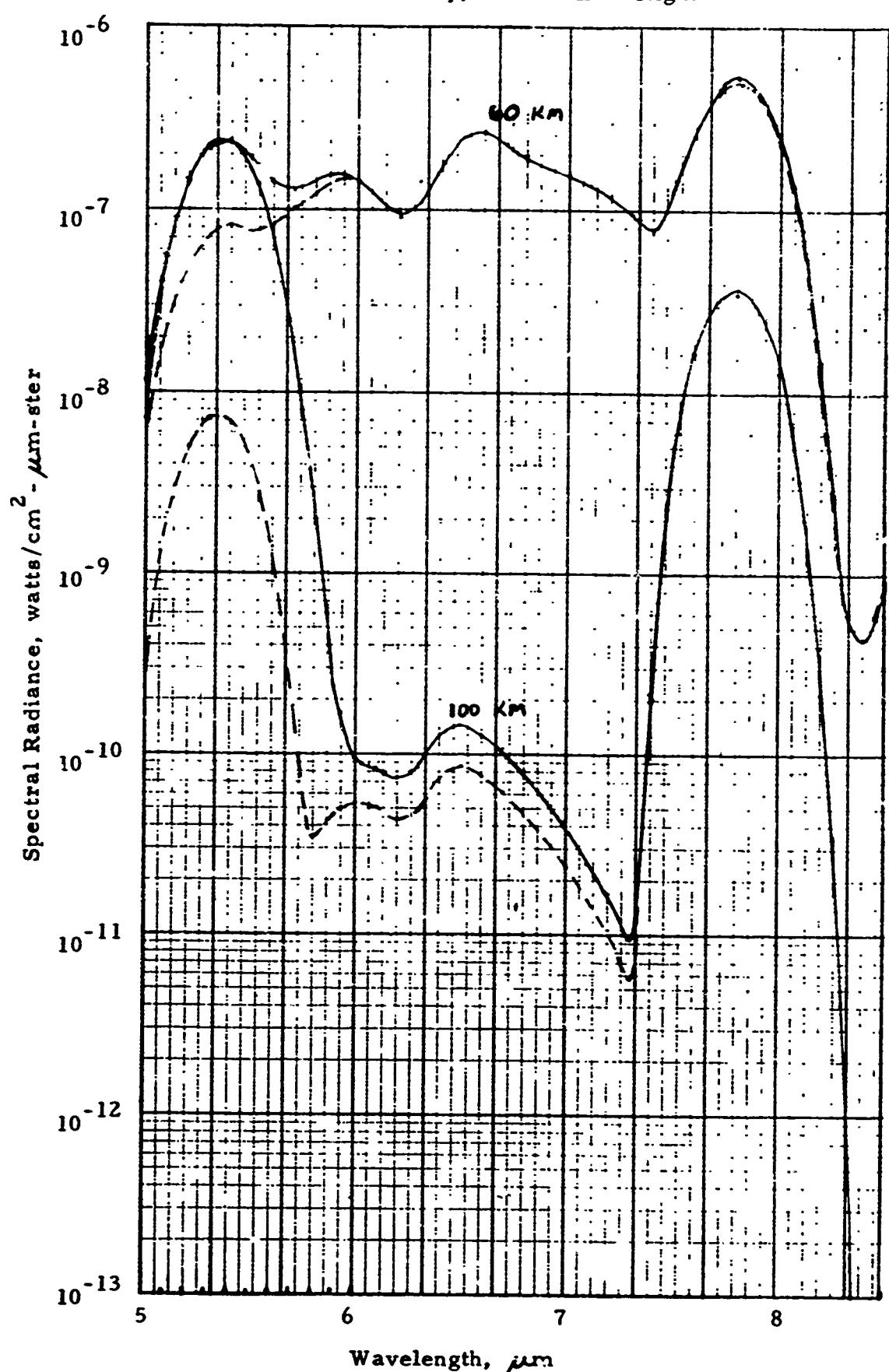


FIGURE V-1

Limb Viewing Spectral Radiances, 8 to 11.5 μm

Solid Line Day, Dashed Line Night

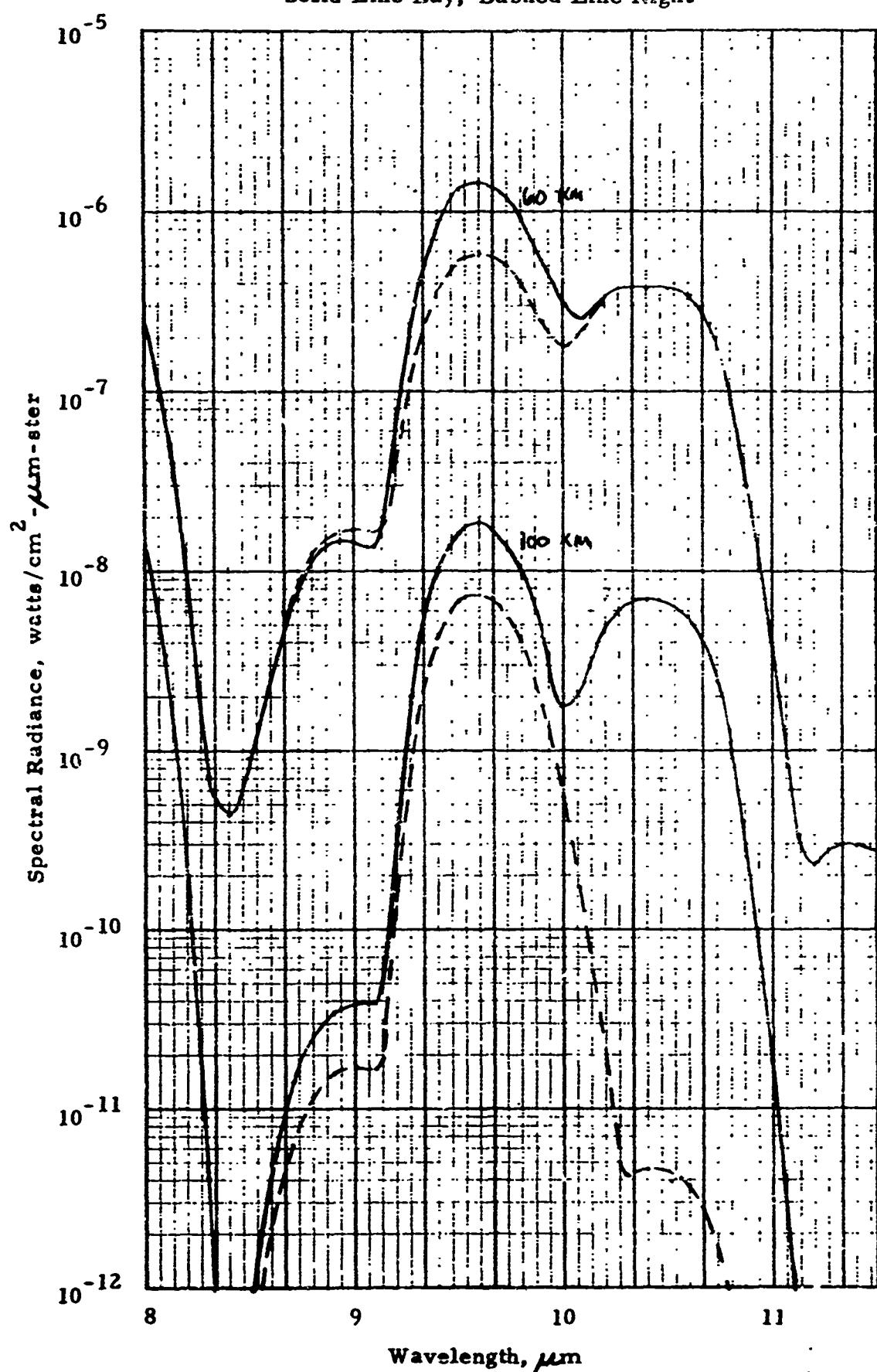
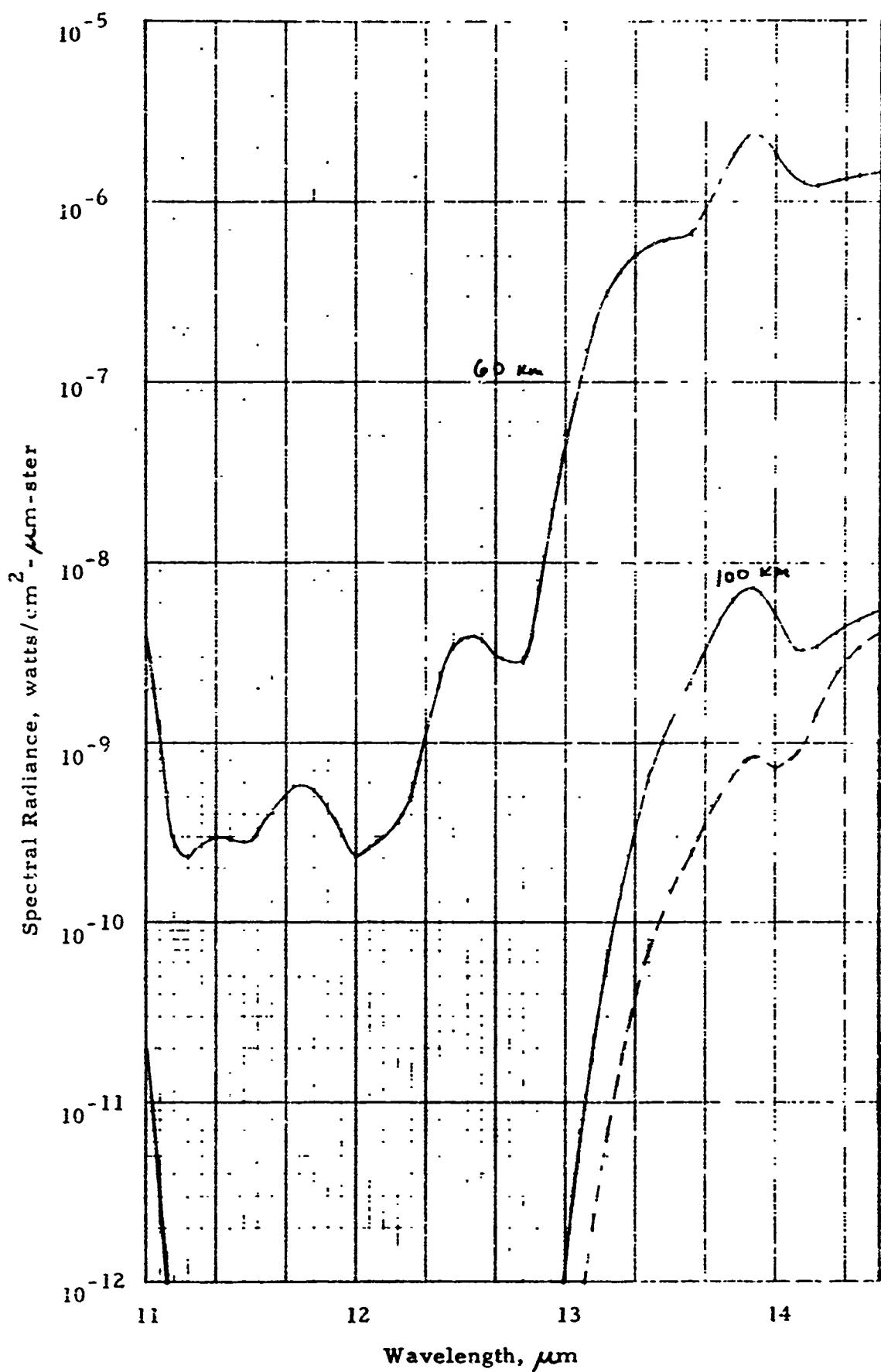


FIGURE V-2

Limb Viewing Spectral Radiances, 11 to 14.5 μm
Solid Line Day, Dashed Line Night



Limb Viewing Spectral Radiances, 14 to 17.5 μm
Solid Line Day, Dashed Line Night

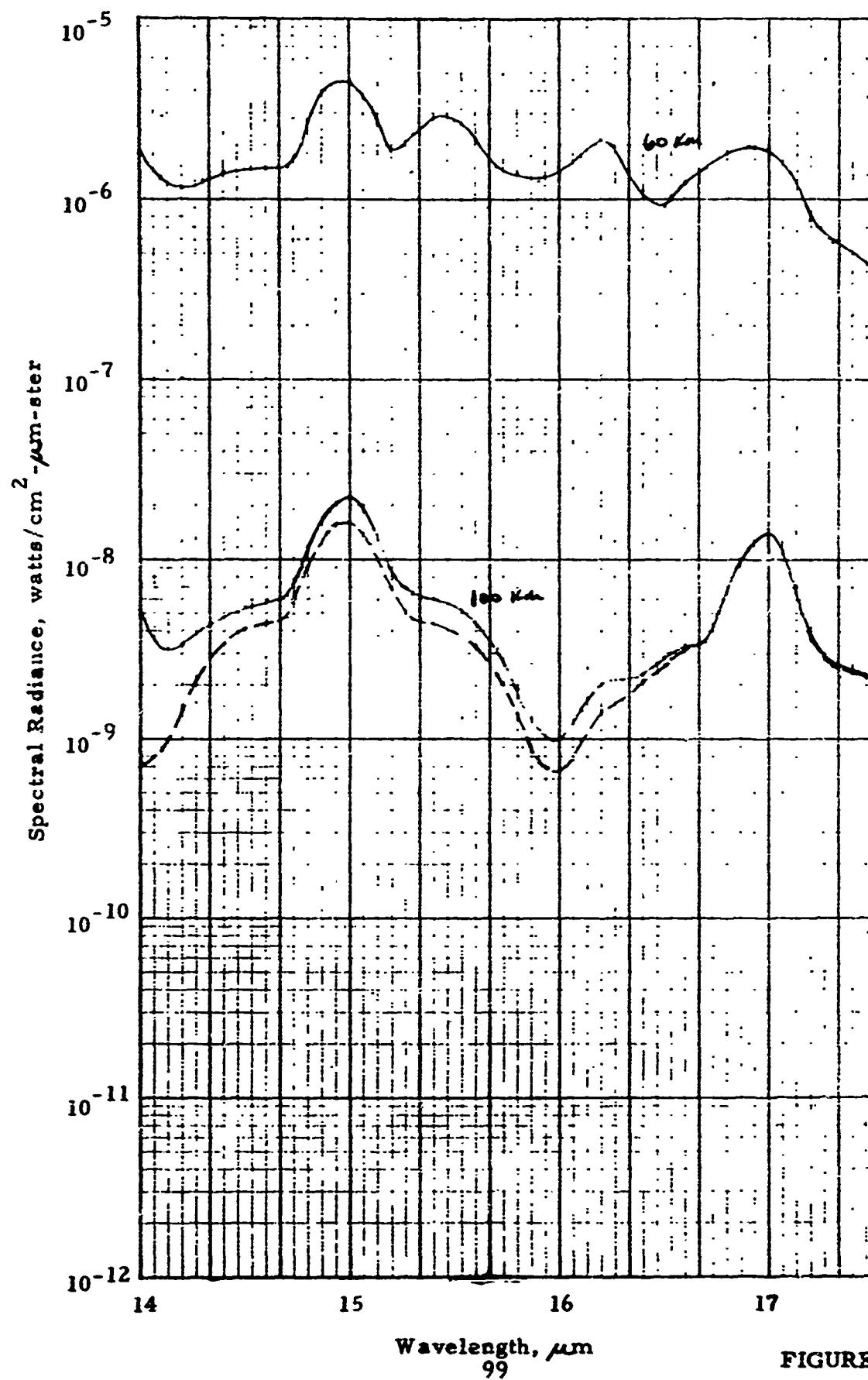
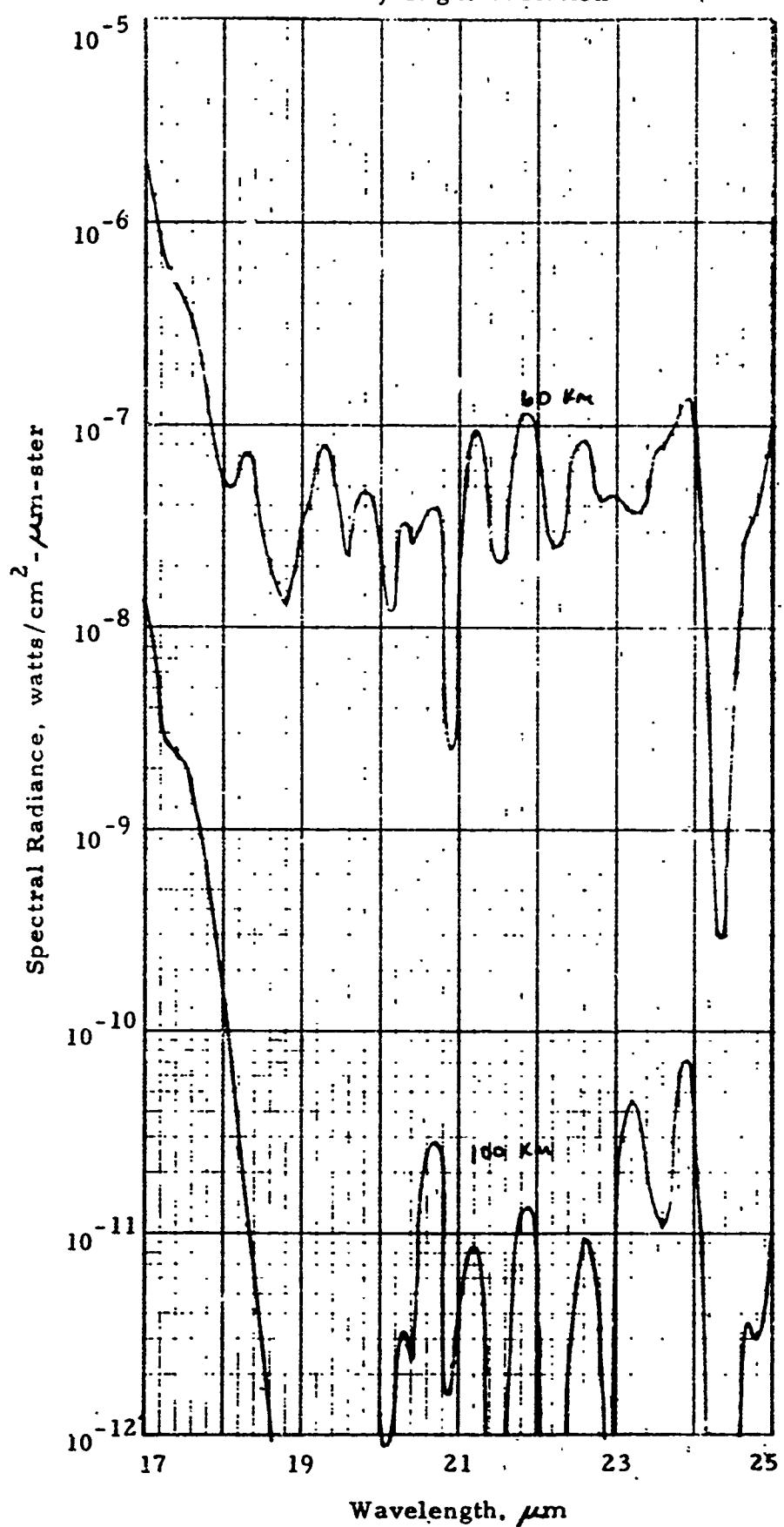


FIGURE V-4

Limb Viewing Spectral Radiances, 17 to 25 μm
No Day-Night Variation



The three general areas of investigation in this research are (a) the chemistry of the upper atmosphere and its relation to production of infrared radiation, (b) the physical mechanisms which excite and quench molecular quantum levels which can radiate in the infrared, and (c) improvement of models of the transport of infrared radiation.

The principal results of the current program have been the development of a program to compute the abundances of infrared emitting molecular species insofar as knowledge of chemical reaction rates permits, and an extension of the limb viewing infrared radiance program of Corbin, et al. (1969). This work is incomplete, but permits the definition of areas in which future work will be profitable.

In principle, especially at the higher altitudes considered here, the chemistry and diffusive mechanisms if properly described should permit the predicted concentrations to approach a diurnal steady-state. That is, the various concentrations should be reattained in every twenty-four hour period. Likewise there should be other steady-state cycle achieved, namely, those varying with the seasons and the 11-year solar cycle. These latter effects require, of course, much more elaborate modeling than is provided in the present context and must consider variation in the total amount of solar energy reaching the various portions of the earth's atmosphere and the large scale wind patterns generated by these variable inputs.

It was not possible in the present program to exercise it sufficiently to allow the diurnal steady state behavior to be investigated over the desired range of altitudes, species, and uncertain reaction rates. One run through a 24-hour cycle was performed over a restricted altitude regime to determine how much the solution varied during a single day from the specified initial conditions. A separate run was performed that covered a total of 12-days real time. These results were not acceptable due to the longer time steps that were required in the program. The exercise of the code must be continued to determine the permissible time steps that will allow steady-state to be

reached within a reasonable machine running time. Investigations must also be made of the effects on this process of the uncertainties in the experimental reaction-rates.

At altitudes above 100 km, the principal source of error in computed limb radiance profiles is the knowledge of molecular abundances. The individual lines in the molecular bands are weak enough that the neglect of collision broadening effects which lead to a Lorentz or similar shape in the wings of lines are negligible. At lower altitudes, the effects of the line wings will increase actual radiances, and further work is required to include this effect in band modeling. The effect of neglecting the far wings of the lines is expected to be greatest in the carbon dioxide bands, and here the problem is complicated by the non-Lorentz wing shape. Further work should be done on band modeling.

Measurements of radiation in spectral regions outside the nominal limits five to twenty-five microns are available and can aid in defining the processes important in producing radiation in that spectral region. The capabilities of the limb viewing atmospheric radiance model should be expanded to include the carbon dioxide and water vapor bands at 2.7 micrometers and other known bands for which sufficient data exists in the spectral range between 2.7 and 25 micrometers. Estimates of global variations of infrared radiation are required and will require at least a qualitative estimate of the effects of horizontal transport (winds, global circulation patterns) on chemistry.

Further work suggested may be summarized in the context of the present problem areas:

Chemistry. The main effort here has been to develop an efficient and reliable program to integrate the photochemical reaction rate equations, including vertical transport by eddy mixing and molecular diffusion, for atmospheric atoms and molecules which radiate in the infrared. At present

eighteen different neutral atoms and molecules are included. These are molecular nitrogen, N_2 , which is treated as a background gas with concentrations determined only by transport; two states of atomic nitrogen, $N(^4S)$ and $N(^2D)$; two states of atomic oxygen, $O(^3P)$ and $O(^1D)$; molecular oxygen, O_2 ; ozone, O_3 ; the hydroxyl radical, OH ; the hydroperoxyl radical, HO_2 ; water vapor, H_2O ; hydrogen peroxide, H_2O_2 ; atomic and molecular hydrogen, H and H_2 ; nitric oxide, NO ; nitrogen dioxide, NO_2 ; methane, CH_4 ; carbon dioxide, CO_2 ; and carbon monoxide, CO . In addition, argon is included to serve as a further check on transport calculations. Running time is slower than desired, and further development should include a search for a more efficient integration scheme, as well as the necessary addition of ionized chemical species. Qualitative estimates of the effects of horizontal transport on atmospheric chemistry should be made.

Excitation Mechanisms. Data on excitation of vibrational levels of infrared emitting molecules by collision with neutral molecules, ionized molecules and electrons need to be continually reviewed. Excitation of vibrational and electronic states of other molecules, particularly nitrogen and metastable states of atomic and molecular oxygen, which can transfer energy to infrared emitting molecules should be included. As relevant new rates are found, they should be added to the chemistry and radiance computer programs.

Radiative Transport Modeling. The addition of new bands requires further modeling of individual bands. The current method should be improved and compared with other methods.

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APPENDIX

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1 (TCX(4),T03), (TCX(5),T0H), (TCX(6),TH), (TCX(7),TH2C), SNAP 370
2 (TCX(8),THC2), (TCX(9),TH202), (TCX(10),TH2), (TCX(11),TCh4), SNAP 380
3 (TCX(12),TC02), (TCX(13),TCC), (TCX(14),TQ1C), (TCX(15),TN), SNAP 390
4 (TCX(16),TN01), (TCX(17),TN02), (TCX(18),TN2C), (TCX(19),TN2C) SNAP 400
C C SNAP 410
      DATA TST /500*0.0/
      DATA TINO /50*10.0,20.0,40.0,80.0,1.0E2,3.0E2,6.0E2,30*1.0E3,
1 1.5E3,2.0E3,2.5E3,3.0E3,3.5E3,4.0E3,4.5E3,5.0E3,5.5E3,6.0E3,
2 1.1E4,1.6E4,2.1E4,2.6E4,3.2E4,3.5E4,3.8E4,4.1E4,4.3E4,4.7E4,
3 395*5.0E4/
      DATA TETOT /50*10.0,20.0,40.0,80.0,1.0E2,3.0E2,6.0E2,26*1.0E3,
1 1.1E3,1.2E3,1.4E3,1.5E3,2.4E3,3.0E3,4.2E3,5.1E3,6.0E3,
2 7.6E3,8.4E3,9.2E3,1.0E4,1.9E4,2.8E4,3.7E4,4.6E4,5.5E4,6.4E4,
3 7.3E4,8.2E4,9.1E4,396*1.0E5/
      DATA TI0 /91*0.0,0.1,0.2,0.3,0.4,0.5,0.7,1.0,1.5,2.5,5.0,
1 10.0,15.0,20.0,25.0,30.0,35.0,40.0,50.0,60.0,80.0,100.0,
2 120.0,140.0,160.0,180.0,220.0,300.0,400.0,500.0,600.0,
3 700.0,750.0,800.0,850.0,900.0,1.0E3,1.0E3,1.4E3,1.4E3,1.6E3,
4 1.8E3,2.0E3,2.2E3,2.4E3,2.7E3,3.0E3,3.5E3,4.0E3,4.5E3,
5 5.0E3,5.5E3,6.0E3,7.0E3,8.0E3,9.0E3,1.0E4,1.1E4,1.2E4,
6 1.3E4,1.4E4,1.5E4,1.6E4,2.1E4,2.4E4,3.0E4,3.3E4,
7 3.6E4,3.9E4,4.2E4,341*4.5E4/
      DATA TI02 /81*0.0,100.0,200.0,300.0,400.0,600.0,900.0,
1 1.2E3,1.6E3,2.0E3,2.5E3,3.1E3,3.4E3,3.7E3,4.0E3,
2 5.0E3,7.0E3,1.0E4,1.5E4,2.0E4,2.3E4,2.6E4,3.2E4,
3 3.5E4,3.8E4,4.1E4,4.4E4,4.7E4,391*5.0E4/
C C SNAP 420
      DATA LALT,LTIME,LCHI,LCOL02,LCOLN2,LJ02,LQ03,LQCOHA,
1 LQCOHB,LQZCHA,LQZCHB,LML /6H ALT,6H TIME ,6H CHI ,6H COL02,
2 6H COLN2,6H COLO3,6H J02 ,6H J03 ,6HQAOH),6HQGB(CHI),6HIA(OH), SNAP E60
3 6HIB(OH),6H ML / SNAP E70
C C SNAP 430
      DATA AMWT / 28.0134, 31.9988, 15.9994, 47.9982, 17.0074,
1 1.00797, 18.0153, 33.0067, 34.0147, 2.01594, 16.0430, 44.0099, SNAP 71
2 28.0105, 15.9994, 14.0067, 30.0061, 46.0055, 44.0128, 14.0067, SNAP 72

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3 39.4480, 36*6.0 /           SNAP 73U
C
C DATA EDC0=F / 51*1.0E5,1.19E5,1.2U2E5,1.318E5,1.445E5,1.565E5,
1.738E5,1.9U5E5,2.0U9E5,2.2U1E5,2.512E5,2.754E5,3.0U2E5,3.31E5,
3.63L5,3.98E5,4.036E5,4.79E5,5.025E5,5.75E5,6.31E5,6.92E5,7.59E5,
8.32E5,9.12E5,1.0E6,1.096E6,1.202E6,1.318E6,1.445E6,1.585E6,
1.738E6,1.905E6,2.0U8E6,2.291E6,2.512E6,2.754E6,3.0U2E6,3.31E6,
3.63E6,3.98E6,4.036E6,4.78E6,5.025E6,5.75E6,6.31E6,6.92E6,7.59E6,
8.32E6,9.12E6,1.0U0E7,1.096E7,1.2U0E7,1.24E7,1.27E7,1.24E7,
1.18E7,1.05E7,8.2U0E6,3.162E6,1.0U0E6,3.162E5,1.00E5,3.162E4,
1.0JE4,3.162E3,1.0U0E3,3.162E2,1.0U0E2,3.162L1,1.0U0E1,3.8U*1.0,
DATA EDCF / 12*1.JE5,7.943E4,6.31U0E4,5.U12E4,3.0U1E4,2.162E4,
2.512E4,1.0295E4,1.0585E4,1.11*1.0E4,1.0259E4,1.0585E4,
2.1.995E4,2.512E4,3.162E4,3.981E4,5.U12E4,6.31U0E4,7.943E4 /
SNAP 850
C DATA LSP /6H   N2   ,6H   0C   ,6H   0(3P),6H   03   ,6H   CH   ,6H   H
1 EH   H20  ,6H   H02  ,6H   H202 ,6H   H2  ,6H   CH4  ,6H   CC2  ,6H   CO  ,
2 EH   0(10),6H   N(4S),6H   NO  ,6H   N02 ,6H   N20 ,6H   N(2C),
3 EH   6H   /
SNAP 860
C DATA TFMT /1UH(/5X,SHSTA,1UHRT,6X,3HEN,1UHD,7X,5*TCT,
1 10HAL,6X,5HT1,10HMES/1X,3F1,5H0.3/)/
SNAP 870
C STATEMENT FUNCTION TC CONVERT DEGREES TO RADIANS
RAU(DEG) = 1.7453292519943E-2*DEG
SNAP 880
C STATEMENT FUNCTION TC COMPLETE 1.0 - EXP(-X)
EXP(X) = (((((0.0J8333*X - 0.04166667)*X + 0.166666666667)*X
1 - U.5)*X + 1.0)*X
SNAP 890
C EDDY DIFFUSION COEFFICIENTS ARE STORED IN ARRAY EDCCEF
C KINETIC TEMPERATURES ARE STORED IN ARRAY TEMFK
C NUMBER DENSITIES FOR ALL ALTITUDES AND SPECIES ARE
C STORED IN ARRAY CONSP
SNAP 900
SNAP 910
SNAP 920
SNAP 930
SNAP 940
SNAP 950
SNAP 960
SNAP 970
SNAP 980
SNAP 990
SNAP 1000
SNAP 1010
SNAP 1020
SNAP 1030
SNAP 1040
SNAP 1050
SNAP 1060
SNAP 1070
SNAP 1080

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C NUMBER DENSITIES FOR ALTITUDE NALT ARE STORED IN ARRAY CCX      SNAP1090
C NUMBER DENSITIES FOR NALT - 1 AT TIME T ARE STORED IN ARRAY SCX      SNAP1100
C ARRAYS RCX AND TCX STORE APPROXIMATIONS DURING INTEGRATION      SNAP1110
C DIFFUSION CONTRIBUTIONS TO THE Q COEFFICIENTS ARE      SNAP1120
C STORED IN ARRAY GJED      SNAP1130
C DIFFUSION CONTRIBUTIONS TO THE BETA COEFFICIENTS ARE      SNAP1140
C STORED IN ARRAY ETED      SNAP1150
C TERMS USED TO COMPUTE QJED ARE STORED IN ARRAYS GJEC AND QJEDU      SNAP1160
C                                     SNAP1170
C                                     SNAP1180
C                                     SNAP1190
C                                     SNAP1200
C                                     SNAP1210
C                                     SNAP1220
C                                     SNAP1230
C                                     SNAP1240
C                                     SNAP1250
C                                     SNAP1260
C                                     SNAP1270
C                                     SNAP1280
C                                     SNAP1290
C                                     SNAP1300
C                                     SNAP1310
C                                     SNAP1320
C                                     SNAP1330
C                                     SNAP1340
C                                     SNAP1350
C                                     SNAP1360
C                                     SNAP1370
C                                     SNAP1380
C                                     SNAP1390
C                                     SNAP1400
C                                     SNAP1410
C                                     SNAP1420
C                                     SNAP1430
C                                     SNAP1440

C INITIALIZATION OF CONSTANTS
NW = 6
NPAGE = -1
PI = 3.1415926535898
RE = 6371.0
DELZ = 1.0E5
ROELZ = 0.5/DELZ
R2DELZ = DELZ**(-2)
NPRINT = 1
DO 90 NALT = 1, 150
EDCOEF(NALT) = EDCOEF(NALT + 9)
90 CONTINUE
DO 95 I = 1, 41
EDCOEF(I) = EDCDF(I)
95 CONTINUE

C FOR CONVENIENCE IN CHECKING FORMATION OF COEFFICIENTS IN THE
C DIFFERENTIAL EQUATIONS, INDEX VALUES OF THE FORM KN2, KO2,
C ETC ARE USED IN PLACE OF SPECIFIC VALUES OF NSF.
KN2 = 1
KO2 = 2
KO = 3
KC3 = 4
KC1 = 5
KH = 6

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SNAF1450
SNAF1460
SNAF1470
SNAF1480
SNAF1490
SNAF1500
SNAF1510
SNAF1520
SNAF1530
SNAF1540
SNAF1550
SNAF1560
SNAF1570
SNAF1580
SNAF1590
SNAF1600
SNAF1610
SNAF1620
SNAF1630
SNAF1640
SNAF1650
SNAF1660
SNAF1670
SNAF1680
SNAF1690
SNAF1700
SNAF1710
SNAF1720
SNAF1730
SNAF1740
SNAF1750
SNAF1760
SNAF1770
SNAF1780
SNAF1790
SNAF1800

KH20 = 7
KH21 = 8
KH202 = 9
KH2 = 10
KCCH4 = 11
KC02 = 12
KC0 = 13
KC01D = 14
KN = 15
KN0 = 16
KN02 = 17
KN20 = 18
KN20 = 19

READ (5,21) IDENT,IDENT
WRITE (4,21) IDENT,IDENT
WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1

      PRINT INPUT PARAMETERS

      WRITE (6,24) IDENT,IDENT
      READ (5,15) OTHETA,CARD
      WRITE (6,15) OTHETA,CARD
      WRITE (4,15) OTHETA,CARD
      READ (5,15) OPHI,CARC
      WRITE (6,15) OPHI,CARC
      WRITE (4,15) OPHI,CARC
      READ (5,15) SCLDEC,CARD
      WRITE (6,15) SOLDEC,CARD
      WRITE (4,15) SOLDEC,CARD
      READ (5,15) GREF,CARC
      WRITE (6,15) GREF,CARC
      WRITE (4,15) GREF,CARC
      READ (5,15) REFF,CARC

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      WRITE (6,15) REFF,CARD
      WRITE (4,15) REFF,CARD
      READ (5,15) EFS,CARD
      WRITE (6,15) EPS,CARD
      WRITE (4,15) EPS,CARD
      READ (5,16) MLMAX,CARD
      WRITE (6,16) MLMAX,CARD
      WRITE (4,16) MLMAX,CARD
      READ (5,16) NBASE,CARD
      WRITE (6,16) NBASE,CARD
      WRITE (4,16) NEASE,CARD
      WRITE (4,16) NEASE,CARD
      READ (5,16) NTOP,CARD
      WRITE (6,16) NTOP,CARD
      WRITE (4,16) NTOP,CARD
      WRITE (4,16) IHRMAX,CARD
      READ (5,16) IHRMAX,CARD
      WRITE (6,16) IHRMAX,CARD
      WRITE (4,16) IHRMAX,CARD
      READ (5,16) MMAX,CARD
      WRITE (6,16) MMAX,CARD
      WRITE (4,16) MMAX,CARD
      READ (5,15) OLTIME,CARD
      WRITE (6,15) CLTIME,CARD
      WRITE (4,15) CLTIME,CARD
      READ (5,15) TIME,CARD
      WRITE (6,15) TIME,CARD
      C ****
      C
      WRITE (6,20) IDENT,NPAGE
      NPAGE = NPAGE + 1
      UO 100 NALT = 1, 201
      READ (5,34) NXX,N1,(CONSP(NALT,J), J = 1, 7)
      WRITE (6,35) NXX,N1,(CONSP(NALT,J), J = 1, 7)
      IF (NXX .NE. NALT) GO TO 500
      IF (N1 .NE. 1) GO TO 500
      READ (5,34) NXX,N2,(CONSP(NALT,J), J = 8, 14)
      C ****
      C
      SNAP1810
      SNAP1820
      SNAP1830
      SNAP1840
      SNAP1850
      SNAP1860
      SNAP1870
      SNAP1880
      SNAP1890
      SNAP1900
      SNAP1910
      SNAP1920
      SNAP1930
      SNAP1940
      SNAP1950
      SNAP1960
      SNAP1970
      SNAP1980
      SNAP1990
      SNAP2000
      SNAP2010
      SNAP2020
      SNAP2030
      SNAP2040
      SNAP2050
      SNAP2060
      SNAP2070
      SNAP2080
      SNAP2090
      SNAP2100
      SNAP2110
      SNAP2120
      SNAP2130
      SNAP2140
      SNAP2150
      SNAP2160
  
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      WRITE (6,35) NXX,N2,(CONSP(NALT,J), J = 8, 14)
      IF (NXX .NE. NALT) GC TO 500
      IF (N2 .NE. 2) GO TO 500
      READ (5,34) NXX,N3,(CONSP(NALT,J), J = 15, 20)
      WRITE (6,35) NXX,N3,(CONSP(NALT,J), J = 15, 20)
      IF (NXX .NE. NALT) GC TO 500
      IF (N3 .NE. 3) GO TO 500
      CONSP(NALT,KN) = 0.1*CONSP(NALT,KN)

100  CONTINUE

      C   INITIALIZE GEOMETRY ROUTINE
      C   CONVERT TO RADIAN MEASURE
      C   OTHETTA=RAD(OTHETA)
      C   OPHI=RAD(OPHI)
      C   SOLDEC=RAD(SOLDEC)
      NSPS = 1
      NSPF = 20
      NGPH = 20
      KTEST = 1
      NBSAV = NBASE

      C   SNAP2 ASSUMES DIFFUSIVE EQUILIBRIUM ABOVE ALTITUDE NTUP
      C   00 450 IHR = 1, IHRMAX
      C   CALL SECOND (SECA)
      C   TIME = TIME + 0.5*DLTIME
      C   WRITE (6,20) IDENT,NPAGE
      C   NPAGE = NPAGE + 1

      C   IF (IHR .EQ. 1) NBASE = 1
      TEMP = 0.0
      TEMP = 0.0
      SHU = 0.0
      SH = 0.0
      GU = 0.0
      G = 0.0
      RHWTU = 0.0

      SNAP2170
      SNAP2180
      SNAP2190
      SNAP2200
      SNAP2210
      SNAP2220
      SNAP2230
      SNAP2240
      SNAP2250
      SNAP2260
      SNAP2270
      SNAP2280
      SNAP2290
      SNAP2300
      SNAP2310
      SNAP2320
      SNAP2330
      SNAP2340
      SNAP2350
      SNAP2360
      SNAP2370
      SNAP2380
      SNAP2390
      SNAP2400
      SNAP2410
      SNAP2420
      SNAP2430
      SNAP2440
      SNAP2450
      SNAP2460
      SNAP2470
      SNAP2480
      SNAP2490
      SNAP2500
      SNAP2510
      SNAP2520

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```

RMWT = 0.0
SLMU = 0.0
SUM = 0.0
I = 0
00 110 NALT = NEASE, NTOP
I = I + 1
NA = NALT - 1
NB = NALT - 2
TEMP = TEMP
TEMP = TEMP
SHL = SH
SH = SHU
GL = G
G = GU
RMWT = RMWT
RMWT = RMWT
SUML = SUM
SUM = SUMU
SUMU = 0.0
RMWTU = 0.0
DD 102 NSP = 1, 20
SUMU = SUMU + CONSP(NALT, NSP)
RMWTU = RMWTU + AMWT(NSP)*CCNSP(NALT, NSP);
CONTINUE
RMWTU = RMWTU/SUMU
RCBS = NA
TEMPU = TKEL(ROBS)
R0TEMPF(NALT) = 2.68684E19*(TEMPU/273.15)+0.75
TEMPK(NALT) = TEMP
GU = GREF*(REFF/(REFF + ROBS))*2
SHU = 8.31432E7*TEMPU/(RMWTU*GU)
IF (I.EQ. 2) SHFACL = EXP(1.0E5/SHU)
IF (I.LE. 2) GC TO 110
IF (NALT.EQ. NTCP - 1) SHFAC = EXP(-1.0E5/SHU)
CTOZ = (TEMPU - TEMP)*RDEL2
DKOZ = (EDCCEF(NALT) - EDCCEF(NB))*RCELZ

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DH0Z = (SHU - SHL)*R2DELZ
TFAC = D1DZ/TFLF
AFAC(NA) = TFAC
SFAC = (4.0 - (TEMU + TEMFL)/TEMP)*R2DELZ + TFAC*TFAC
BFAC(NA) = SFAC
FAC = 1.0/SH + TFAC
EC = EDCDEF(NA)
BTEC(NA) = (SFAC + DH0Z/(SH*SH))*ED - FAC*D0DZ
CFAC(NA) = (TEMFL/GU - TEMP/CL)*G + G*R2DELZ/(8.31432E7*TEMP)
DFAC(NA) = G/(8.31432E7*TEMP)
FAC = (FAC*ED + CKCZ)*R2DELZ
QJEDU(NA) = R2CELZ*ED + FAC
QJEDL(NA) = R2CELZ*ED - FAC
IF (IHR .GT. 1) GC(11)
CONFAC = SUML*(QJEDL(NA)/QJEDU(NA) + 1.0)/((BTEC(NA)/QJEDU(NA)
1 + (TEMU - TEMFL)/TEMP + 2.0*R2DELZ/SH)*SUM)
SUM = CONFAC*SUML
IF (NALT .EQ. NTCF) CCN = (BTEC(NA)*SUM - QJEDL(NA)*SUML)
1 / (QJEDU(NA)*SUML)
00 104 NSP = 1, NSPM
CCNSF(NA,NSF) = CCNSP(NA,NSF)*CONFAC
IF (NALT .EQ. NTCF) CCNSP(NTCF,NSP) = CON*CONF(NTCF,NSF)
CONTINUE
104
1 WRITE(6,6) NE,CCNSP(NA,1),CCNSF(NA,2),GL,SH,CTCZ,CKCZ,DH0Z,
  1 9TEC(NA),QJEDL(NA),QJEDU(NA)
  1 WRITE(6,6) N1,PMWT,TFAC,SFAC,CFAC(NA),DFAC(NA),RDTEMP(NA)
  1 WRITE(6,6) NALT,CCNC(1),CCNC(2),CONC(4),CCNC(7),CCNC(9),CCNC(10)
CONTINUE
110
NEASE = NBSAV
NEASE = NEASE + 1
NTOP = NTOP - 1
NMIN = NBASE - 1
CC 410 M = 1, MAX
NTIME = (0.5*CLTIME + TIME)/60.0 + 720.1
RTIME = FLOAT(INTIME)/60.0
NTIME = 1.0*(INTIME/60) + MOD(INTIME,60)
SNAP28
SNAP291
SNAP292
SNAP293
SNAP294
SNAP295
SNAP296
SNAP2970
SNAP2980
SNAP2990
SNAP3000
SNAP3010
SNAP3020
SNAP3030
SNAP3040
SNAP3050
SNAP3060
SNAP3070
SNAP3080
SNAP3090
SNAP3100
SNAP3110
SNAP3120
SNAP3130
SNAP3140
SNAP3150
SNAP3160
SNAP3170
SNAP3180
SNAP3190
SNAP3200
SNAP3210
SNAP3220
SNAP3230
SNAP3240

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```

IF (MC0(M,NPRNT) .NE. 0) GO TO 120
WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1
WRITE (6,6) NTIME,RTIME
WRITE (6,19)
C      WRITE (6,22) LALT,LTIME,LCHI,LCOL02,LCOLN2,LCCCLC3,LJC2,LJO?
      WRITE (6,22) LALT,LQCCHA,LGCCCH8,LQZCHA,LOZOHB,((LSP(I),I=1,E)
      WRITE (6,22) LPL,(LSP(I),I=7,14)
      WRITE (6,19)
CONTINUE
120      RFAC = ROTEMP(NMIN)
C1 = CONSP(NMIN,1)
C2 = CONSP(NMIN,2)
C3 = CONSP(NMIN,3)
CMOL(1) = RFAC/(C1/0.180 + C2/0.181 + C3/0.260)
CMOL(2) = RFAC/(C1/0.181 + C2/0.189 + C3/0.260)
CMOL(3) = RFAC/(C1/0.260 + C2/0.260 + C3/0.370)
RFAC = ROTEMP(NBASE)
C1 = CONSP(NBASE,1)
C2 = CONSP(NBASE,2)
C3 = CONSP(NBASE,3)
CMD(1) = RFAC/(C1/0.180 + C2/0.181 + C3/0.260)
CMD(2) = RFAC/(C1/0.181 + C2/0.189 + C3/0.260)
CMD(3) = RFAC/(C1/0.260 + C2/0.260 + C3/0.370)
DO 130 NSP = 1,NSPM
SCX(NSP) = CONSP(NBASE-1,NSP)
IF (NSP .LT. 4) GO TO 130
CMOL(NSP) = U.707*CMOL(2)*SQRT((31.9988/AMWT(NSP) + 1.0)
CMD(NSP) = U.707*CMD(2)*SQRT((31.9988/AMWT(NSP) + 1.0)
CONTINUE
130      DZOMA = 0.0
DZOMB = 0.0
DO 350 NALT = NBASE, NTOP
NPLU = NALT + 1
NAMIN = NALT - 1
RFAC = ROTEMP(NPLU)

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C1 = CJNSP(NPLU,1)           SNAP3E10
C2 = CONSP(NFLL,2)           SNAF3E20
C3 = CONSP(NPLU,3)           SNAF3E30
CNDU(1) = RFAC/ (C1/U*181 + C2/U*181 + C3/U*260) SNAP3E40
CNDU(2) = RFAC/ (C1/U*181 + C2/U*189 + C3/U*260) SNAP3E50
CNDU(3) = RFAC/ (C1/U*261 + C2/U*260 + C3/U*370) SNAP3E60
AFACNA = AFAC(NALT)         SNAP3E70
BFACNA = BFAC(NALT)         SNAP3E80
CFACNA = CFAC(NALT)         SNAP3E90
DFACNA = DFAC(NALT)         SNAP3700
QJEDUN = QJEDU(NALT)        SNAP3710
QJEDLN = QJEDL(NALT)        SNAP3720
BTEDNA = BTED(NALT)         SNAP3730
00 14U NSP = 1,NSP          SNAP3740
CCNSPN = CONSP(NALT,NSP)    SNAP3750
DCX(NSP) = CONSPN           SNAP3760
TCX(NSP) = CONSPN           SNAP3770
CNDNSP = CND(NSP)           SNAP3780
IF (NSP .LT. 4) GO TO 135
CNDU(NSP) = U.707*CNDU(2)*SCRT(31.9988/AMWT(NSP) + 1.0)
135  CONTINUE
      FAC = AMWT(NSP)*CFACNA + AFACNA
      DDDZ = (CNDU(NSP) - CND(NSP))*RDELZ
      BTEND(NSP) = (BFACNA + AMWT(NSP)*CFACNA)*CNDNSP - FAC*OCCZ
      1 + BTENDNA
      FAC = (FAC*CNDNSF + OCCZ)*RDELZ
      QJEMD(NSP) = (RDELZ*CNDNSP + FAC + QJEDUN)*CCNSF(NFLU,NSP)
      1 + (RDELZ*CNDNSF - FAC + QJELLN)*CNSP(NAMIN,NSF)
      CND(NSP) = CNDNSP
      CND(NSP) = CND(NSP)
      CONTINUE
      TEMP = TEMPK(NALT)
      RCBS = FLOAT(NALT - 1)
      CALL SOLLY(DTHETA,ROES,TIME,SOLDEC,CHI,ETA)
      IF (ETA .LE. 0.0) GO TO 160
      CHISAV = 1.0

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SNAP3E70
SNAP3E80
SNAP3E90
SNAP4000
SNAP4010
SNAP4020
SNAP4030
SNAP4040
SNAP4050
SNAP4060
SNAP4070
SNAP4080
SNAP4090
SNAP4100
SNAP4110
SNAP4120
SNAP4130
SNAP4140
SNAP4150
SNAP4160
SNAP4170
SNAP4180
SNAP4190
SNAP4200
SNAP4210
SNAP4220
SNAP4230
SNAP4240
SNAP4250
SNAP4260
SNAP4270
SNAP4280
SNAP4290
SNAP4300
SNAP4310
SNAP4320

145  CONTINUE
      CALL COLUMN (ROBS,CHI,COL,ETA)
      COL(1) = CHISAV*COL(1)
      COL(2) = CHISAV*COL(2)
      COL(3) = CHISAV*COL(3)
      COL(4) = CHISAV*COL(4)
      CONTINUE
150  CONTINUE
      CALL SUNPHI (COL,ETA,RATE)
      TEMP1 = 1.0/TEMP
      TEMP12 = SQRT (TEMP1)
      TEMP32 = TEMP1*TEMP12
      TEMP52 = TEMP1*TEMP32
      FORWARD REACTIONS
      REVERSE REACTIONS
      C REACTION 1 N + O2 = NO + C
      R1 = 1.1E-14*TEMP*EXP(-3140.0*TEMP1)
      S1 = 2.6E-15*TEMP*EXP(-19500.0*TEMP1)
      C REACTION 2 N + NO = N2 + C
      R2 = 5.1E-11*EXP(-168.0*TEMP1)
      S2 = 2.3E-10*EXP(-37500.0*TEMP1)
      C REACTION 3 NO + NO = N2 + C2
      R3 = 1.3*TEMP52*EXP(-42800.0*TEMP1)
      S3 = 15.2*TEMP52*EXP(-64300.0*TEMP1)
      C REACTION 4 O + O + M = O2 + M
      R4 = 3.8UE-30*TEMP1*EXP(-171.0*TEMP1)
      S4 = 4.57E-5*TEMP1*EXP(-59700.0*TEMP1)
      C REACTION 5 N + N + M = N2 + M
      R5 = 1.4E-33*EXP(-500.0*TEMP1)
      S5 = 3.2E-7*TEMP12*EXP(-112000.0*TEMP1)
      C REACTION 6 N + N + N2 = N2 + N2
      R6 = 7.3E-32*TEMP12
      S6 = 7.8E-7*TEMP12*EXP(-112000.0*TEMP1)

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C   REACTION 7  N + N + N = N2 + N
C   R7 = 2.5E-27*TEMP32
C   S7 = 6.75E-2*TEMP32*EXP(-1126.00*TEMP1)
C   REACTION 8  N + C + M = NC + M
C   R8 = 1.1E-32*SGRT(273.0*TEMP1)
C   S8 = 3.8E-7*TEMP12*EXP(-74500.0*TEMP1)
C   REACTION 9  NC + O = NC2 + F-NU
C   R9 = 6.5E-17*TEMP/296.0
C   S9 = RATE(4)
C   REACTION 10  C + NO2 = NO + C2
C   R10 = 1.6E-11*EXP(-300.0*TEMP1)
C   S10 = 1.0E-37
C   REACTION 11  N + NO2 = N2 + O2
C   R11 = 2.3E-12
C   S11 = 1.0E-37
C   REACTION 12  N + NO2 = NO + NO
C   R12 = 5.9E-14
C   S12 = 1.0E-35
C   REACTION 13  NO + O + M = NC2 + M
C   R13 = 2.9E-33*EXP(940.0*TEMP1)
C   S13 = 1.8E-8*EXP(-32800.0*TEMP1)
C   REACTION 14  NO + NC + O2 = NO2 + NC2
C   R14 = 6.6E-39*EXP(530.0*TEMP1)
C   S14 = 6.6E-12*EXP(-1350.0*TEMP1)
C   REACTION 15  O + C = O2 + F-NU
C   S15 = RATE(1)
C   REACTION 16  N + O = NO + F-NU
C   S16 = RATE(3)
C   REACTION 21  NC + O3 = O2 + NC2
C   R21 = 9.5E-13*EXP(-1240.0*TEMP1)
C   S21 = 1.0E-13*EXP(-2350.0*TEMP1)
C   REACTION 31  O + O2 + M = C3 + M
C   R31 = 4.63E-35* EXP(1060.00*TEMP1)
C   S31 = 1.65E-9* EXP(-11920.0*TEMP1)
C   REACTION 32  C + C3 = O2 + C2
C   R32 = 2.0E-11* EXP(-2410.0*TEMP1)

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S32 = 2.12E-11*EXP(-50700.0 * TEMPI)
REACT1CN 33 H + O3 = OH + C2
R33 = 2.6E-11
S33 = 0.
REACT1CN 34 O + OH = H + C2
R34 = 2.06E-11
S34 = 4.19E-10 * EXP(-8450.0 * TEMPI)
R35 H02 + O = OH + C2
R35 = 1.0E-11
C R36 H02 + H == OH + CH
R36 = 2.0E-10*EXP(-2000.0*TEMPI)
C R37 H + O2 + H = H02 + H
R37 = 3.0E-32*(273.0*TEMPI)**1.3
C R38 OH + C3 = HC2 + O2
R38 = 5.0E-13
C R39 H02 + O3 = OH + O2 + C2
R39 = 1.0E-14
C R40 OH + CH = H2C + O
R40 = 9.36E-12*EXP(-390.0*TEMPI)
C S40 = 9.3E-11*EXP(-900.0*TEMPI)
C R41 OH + H02 = H2O + O2
R41 = 1.0E-11
C R42 H + HC2 = H2 + C2
R42 = 2.0E-13
C R43 O + H2 = CH + H
R43 = 7.0E-11*EXP(-5100.0*TEMPI)
C R44 H02 + H02 = H2O2 + O2
R44 = 1.5 E-12
C R45 OH + H2C2 = H2O + H02
R45 = 4.0E-13
C R46 O + H2C2 = OH + H02
R46 = 1.0E-15
C R47 H + H2O2 = H2 + H02
R47 = 1.0E-13
C R50 O(ID) + C3 = O2 + O2
R50 = 5.0E-11
SNAP4600
SNAP4700
SNAP4710
SNAP4720
SNAP4730
SNAP4740
SNAP4750
SNAP4760
SNAP4770
SNAP4780
SNAP4790
SNAP4800
SNAP4810
SNAP4820
SNAP4830
SNAP4840
SNAP4850
SNAP4860
SNAP4870
SNAP4880
SNAP4890
SNAP4900
SNAP4910
SNAP4920
SNAP4930
SNAP4940
SNAP4950
SNAP4960
SNAP4970
SNAP4980
SNAP4990
SNAP5000
SNAP5010
SNAP5020
SNAP5030
SNAP5040

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C      R51  O(ID) + N2 = O + N2
C      R51 = 5.0E-11
C      R52  O(ID) + H2 = OH + H
C      R52 = 1.0E-11
C      R53  O(ID) + H2O = OH + OH
C      R53 = 3.0E-11
C      R54  O(ID) + CH4 = PRODUCTS
C      R54 = 1.0E-11
C      R55  CH4 + OH = H2O + CH3
C      R55 = 1.2E-10*EXP(-2960.0*TEMP1)
C      R56  O + CH4 = CH + CH3
C      R56 = 3.5E-11*EXP(-4550.0*TEMP1)
C      R60  CO + OH = CO2 + H
C      R60 = 1.0E-12*EXP(-540.0*TEMP1)
C      R61  CO + C + H = CO2 + H
C      R61 = 1.4E-33*EXP(-1250.0*TEMP1)
C      IONIC REACTION 1  O2+ + E = C + O
C      RX1 = 6.0E-5*TEMP1
C      SI1 = 0.0
C      IONIC REACTION 2  N2+ + E = N + N
C      RI2 = 5.0E-5*TEMP1
C      SI2 = 0.0
C      IONIC REACTION 3  N2+ + O2 = N2 + O2+
C      RI3 = 1.0E-10
C      SI3 = 0.0
C      IONIC REACTION 4  N2+ + E = N2 + H-NU
C      RI4 = 1.0E-16
C      SI4 = 1.0E-16
C      WRITE (6,19)
C      NA = NALT - 1
C
C      170. CONTINUE
C
C      CO 300 ML = 1, MLMAX

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BTT = S4*XM4 + R31*XM31*T0 + (S34 + R37*XM37)*TH + RATE(1) SNAP5770
QJT = ((R32*T0 + R39*TH02 + R50*T01C)*2.0 + RATE(5) SNAP5780
1 + S31*XM31 + R33*TH + R38*TCH) * T03 SNAP5790
2 + (R4*XM4*T0 + R34*TCH + R35*TH02) * T0 SNAP5800
3 + (R41*TOH + R42*TH + R44*TH02) * TH02 SNAP5810
GC TO 251 SNAP5820
SNAP5830
SNAP5840
SNAP5850
SNAP5860
SNAP5870
SNAP5880
SNAP5890
SNAP5900
SNAP5910
SNAP5920
SNAP5930
SNAP5940
SNAP5950
SNAP5960
SNAP5970
SNAP5980
SNAP5990
SNAP6000
SNAP6010
SNAP6020
SNAP6030
SNAP6040
SNAP6050
SNAP6060
SNAP6070
SNAP6080
SNAP6090
SNAP6100
SNAP6110
SNAP6120

C ATOMIC OXYGEN, O(3P)
C 203 CONTINUE
APT = 2.0*R4*XM4
BTT = R31*XM31*T02 + R32*T03 + R34*TOH + R35*THC2
1 + R43*TH2 + R46*TH202 + R56*TCH4 + R61*XM61*TCC
QJT = (2.0*S4*XM4 + S32*T02 + S34*TH + RATE(8))*TC2
1 + (S31*XM31 + RATE(10))*TC3 + R40*TOH*TOH + R51*TN2*T010
GO TO 251

C OZONE
C 204 CONTINUE
APT = 0.0
BTT = S31*XM31 + R32*T0 + R33*TH + R38*TOH + R39*THC2
1 + R50*T01D + RATE(5)
QJT = (R31*XM31*T0 + S32*T02) * T02
GC TO 251

C HYDROXYL
C 205 CONTINUE
APT = 2.0*R40
ETT = R34*T0 + R38*T03 + R41*TH02 + R45*TH202 + R60*TC0
1 + R55*TCH4
QJT = (R35*TH02 + R43*TH2 + R46*TH202 + R56*TCH4)*TC
1 + (R52*TH2 + 2.0*R53*TH20 + R54*TCH4)*T010 + R39*THC2*TC3
2 + (R33*T03 + S34*T02 + 2.0*R36*TH02)*TH + 2.0E-5*RATE(5)*TH202
3 + RATE(6)*TH20
GO TO 251

C ATOMIC HYDROGEN

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206 CCNTINUE
 APT = 0.0
 BTT = (S34 + R37*XM37)*T02 + (R42 + R36)*TH02 + R33*T03
 1 + R47*TH202
 QJT = (R34*TOH + R43*TH2)*TC + R52*T01D*TH2 + R60*TCH*TCC
 1 + RATE(6)*TH20 + RATE(7)*TCH4
 GO TO 251

C WATER VAPOR
 207 CONTINUE
 APT = 0.0
 BTT = R53*TC1C + RATE(6)
 QJT = (R40*TCH + R41*TH02 + R45*TH2C2 + R55*TCH4)*TCH
 GO TO 251

C PEROXYXYL
 208 CONTINUE
 APT = 2.0*R44
 BTT = R35*TC + R39*T03 + R41*TOH + (R36 + R42)*TH
 QJT = (R45*TOH + R46*T0 + R47*TH)*TH202 + R38*TCH*TCC
 1 + R37*XM37*TH*T02
 GO TO 251

C HYDROGEN PEROXIDE
 209 CONTINUE
 APT = 0.0
 BTT = R45*TOH + R46*TC + R47*TH + 1.0E-2*RATE(5)
 QJT = R44*TH02*THC2
 GO TO 251

C MOLECULAR HYDROGEN
 210 CONTINUE
 APT = 0.0
 BTT = R43*TC + R52*T01D
 QJT = (R42*TH02 + R47*TH202)*TH
 GO TO 251

133

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C   C   METHANE
C   211  CONTINUE
      AFT = 0.0
      BTT = RATE(7) + R54*TC10 + R55*T0
      QJT = 0.0
      GO TO 251

C   C   CARBON DIOXIDE
C   212  CONTINUE
      AFT = 0.0
      BTT = RATE(2) + 1.0E-9*ETA*TIO(NALT)
      XXX12 = R60*T0H + R61*XM61*TC
      QJT = XXX12*TCC
      GO TO 251

C   C   CARBON MONOXIDE
C   213  CONTINUE
      AFT = 0.0
      BTT = XXX12
      QJT = (RATE(2) + 1.0E-9*ETA*TIO(NALT))*TC02
      GO TO 251

C   C   ATOMIC OXYGEN, O(1D)
C   214  CONTINUE
      AFT = 0.0
      BTT = R50*TC3 + R51*TH2 + R52*TH2 + R53*TH20 + R54*TC4
      QJT = RATE(2)*TCC2 + FATE(9)*T02 + FATE(11)*TC3
      GO TO 251

C   C   ATOMIC NITROGEN, N(4S)
C   215  CONTINUE
      QJT = ((S5*XM5 + S6*TH2 + S7*T0) * 2.0 + S2*T0
      1 + S1*T02) * TN2 + (S1*T0 + S8*XM8 + S12*TNC + S16) * TNO
      3 + 1.0E-14*TN2*TN2C
      BTT = (R11 + R12) * TN02 + R8*XM8*T0 + R2*TNO + R1*TC2

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APT = (R5*XH5 + R6*TN2 + R7*TN)*2.0
GO TO 251

C- C- NITRIC OXIDE
216 CONTINUE
1 QJT = ((R12*TN + S14*TN02)*2.0 + S9 + R10*T0
1 + S13*XH13)*TN02 + (R1*T02 + R8*XH8*T0)*TN
2 + (S2*T0 + 2.0*S3*T02)*TN2
3 + 5.0E-12*TN20*T02
BTI = (R13*XH13 + R9 + S1)*TC + R2*TN + R21*TC3
1 + S8*XH8 + S10*T02 + S16
2 + 0.1*RATE(7)
APT = (R14*T02 + S12 + R3)*2.0
GO TO 251

C- C- NITROGEN DIOXIDE
217 CONTINUE
1 QJT = ((2.0*R14*TNO + R43*XH13 + R9)*T0 + R21*TC3
1 + S12*TNO + S10*T02)*TNO + S11*TN2*T02
BTI = (R11 + R12)*TN + S9 + R10*T0 + S13*XH13
APT = 0.0
GO TO 251

C- C- NITROUS OXIDE
218 CONTINUE
1 QJT = 0.0
BTI = 0.0
APT = 0.0
GO TO 251

C- C- ATOMIC NITROGEN, N(2C)
219 CONTINUE
1 QJT = 1.5E-4*TEMPI*ETA*TINO(NALT)*TETOT(NALT)
BTI = 1.0E-14*TN2 + 5.0E-12*T02
APT = 0.0
GO TO 251

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SNAP7210
SNAP7220
SNAP7230
SNAP7240
SNAP7250
SNAP7260
SNAP7270
SNAP7280
SNAP7290
SNAP7300
SNAP7310
SNAP7320
SNAP7330
SNAP7340
SNAP7350
SNAP7360
SNAP7370
SNAP7380
SNAP7390
SNAP7400
SNAP7410
SNAP7420
SNAP7430
SNAP7440
SNAP7450
SNAP7460
SNAP7470
SNAP7480
SNAP7490
SNAP7500
SNAP7510
SNAP7520
SNAP7530
SNAP7540
SNAP7550
SNAP7560

C 220 CONTINUE
QJT = 0.0
BTT = 0.0
APT = 0.0
GO TO 251

C 221 CONTINUE
GO TO 253
BTT = BTT + BTEM0(NSP)
QJT = QJT + QJEM0(NSP)
IF (APE .LE. 0.0) GO TO 252
FAC4AC = 4.0 * APT * QJT
BTSQ = BTT * BTT
FACRT = FAC4AC / BTSQ
DLT = SQRT(FAC4AC + BTSQ)
FACDMB = DLT - BTT
IF (FACRT .LT. 0.01) FACDMB = (((((0.027344 - 0.0205 * FACRT)
* FACRT - 0.0390625) * FACRT + 0.0625) * FACRT - 0.125) * FACRT)
+ 0.5) * FACRT * BT
FAC2AX = 2.0 * APT * OCT
FACB = DLT * OCTIME
FAC = EXP(CAMAX1(-675.0, AMIN1((-FACB, 675.0))))
FAC = 1.0 - FAC
IF ((FACB .LT. 0.01) FACM = EXPM(FACB))
RCX(NSP) = (((BTT + DLT) * FAC + FACDMB) * CCT + 2.0 * QJT * FACM)
1 / ((FAC2AX + BTT) * FACM + (FAC + 1.0) * DLT)
2

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      GO TO 253
252  CONTINUE
      FACB = EXP(AWAX1(-675.0,AMIN1(-FACB,675.0)))
      FACM = 1.0 - FAC
      IF (FACB .LT. 0.01)  FACM = EXPM(FACB)
      RCX(NSP) = OCT*FAC + FACM*GJ1/BTT
      CONTINUE
253  CONTINUE
      ITER = ITER + 1
      IF (ITER .GT. 2) GO TO 260
      DO 258 NSP = 1, NSPM
      TCX(NSP) = RCX(NSP)
258  CONTINUE
      DTIME = 2.0*DTIME
      IF (ITER .EQ. 2) GC TC 200
      CONTINUE
260  CONTINUE
      DO 260 NSP = 1, NSPM
      DCX(NSP) = ABS(RCX(NSP))
260  CONTINUE
      DO 270 NSP = 1, NSPM
      DCX(NSP) = ABS(RCX(NSP))
270  CONTINUE
      DO 280 NSP = 1, NSPM
      DCX(NSP) = ABS(RCX(NSP))
280  CONTINUE
      DO 290 NSP = 1, NSPM
      DCX(NSP) = ABS(RCX(NSP))
290  CONTINUE
      IF (MLMAX .EQ. 1) GO TO 310
      CALL R0MTST (ML,NSPM,CCX,TST,TCX,KTEST,EPS)
      IF (KTEST .EQ. 0) GO TC 310
      CONTINUE
300  CONTINUE
      ML = 100*KTEST + MLSAVE
      MLPRTN(MLALT) = ML
      IF (KTEST .EQ. 0) GO TO 310
      DO 315 NSP = 1, NSPM
      TCX(NSP) = RCX(NSP)
315  CONTINUE
      DO 318 CCNTINUE
      DO 320 NSP = 1, NSPM
      CCNSP(NAMIN,NSP) = SCX(NSP)
320  CONTINUE

```

```

SCX(NSP) = ABS(TCX(NSP))
IF (NALT .EQ. NTOP) CONSP(NALT,NSP) = SCX(NSP)

1   CONSP(NPLU,NSP) = SCX(NSP)*EXP(-1.0E5*AMWT(NSP)*CFACNA)

320  CONTINUE
    QCOHA = R33*TCX(KH)*TCX(K03)
    QCOHB = R35*TCX(KH02)*TCX(KC)
    OZ0HA = OZ0HA + 1.0E5*QCOHA
    OZ0HB = OZ0HB + 1.0E5*QCOHB
    IF (M00(M,NPRNT) .NE. 0) GC TO 35U
    WRITE (6,6) NA,QCOHA,CCOHB,C20HA,OZCHB,(TCX(I),I=1,6)
    WRITE (6,6) ML,(TCX(I),I=7,16)
    CONTINUE
    IF (M00(M,NPRNT) .EQ. 0)
        1  WRITE (6,30) (MLPRNT(I), I = NBASE, NTOP)
    TIME = TIME + DLTIME
    IF (TIME .GT. 4.32E4) TIME = TIME - 8.64E4

400   CONTINUE
    TIME = TIME - 0.5*DLTIME
    WRITE (4,15) TIME,CARD
    NB = NBASE - 1
    NT = NTOP + 1
    DO 420 NALT = 1, NT
    WRITE (4,34) NALT,N1,(CONSP(NALT,I), I = 1, 7)
    WRITE (4,34) NALT,N2,(CONSP(NALT,I), I = 8, 14)
    WRITE (4,34) NALT,N3,(CONSP(NALT,I), I = 15, 20)
    CONTINUE
    IS = 1
    DO 440 IP = 1, 2
    IF = 13 + 9
    NS = 1
    DO 435 IX = 1, 5
    NF = NS + 50
    WRITE (6,20) IDENT,NPAGE
    NPAGE = NPAGE + 1
    WRITE (6,6) NTIME,RTIME
    SNAP7E30
    SNAP7E40
    SNAP7E50
    SNAP7E60
    SNAP7E70
    SNAP7E80
    SNAP7990
    SNAP8000
    SNAP8010
    SNAP8020
    SNAP8030
    SNAP8040
    SNAP8050
    SNAP8060
    SNAP8070
    SNAP8080
    SNAP8090
    SNAP8100
    SNAP8110
    SNAP8120
    SNAP8130
    SNAP8140
    SNAP8150
    SNAP8160
    SNAP8170
    SNAP8180
    SNAP8190
    SNAP8200
    SNAP8210
    SNAP8220
    SNAP8230
    SNAP8240
    SNAP8250
    SNAP8260
    SNAP8270
    SNAP8280

```

```

      WRITE (6,19) LALT, (LSF(I), I = IS, IF)
      WRITE (6,19)
      DO 430 NALT = NS, NF
      NA = NALT - 1
      WRITE (6,6) NA, (CONSP (NALT,I), I = IS, IF)
      CONTINUE
      NS = NF
      CONTINUE
      IS = 11
      CONTINUE
      NBASE = NBASE - 1
      NTOP = NTOP + 1
      CALL SECOND (SECB)
      SECC" = SEC8 - SECA
      WRITE (NH,TFMT) SECA, SEC8, SECC
      CONTINUE
      WRITE (6,20) IDENT, NPAGE
      NPAGE = NPAGE + 1
      CONTINUE
      WRITE (6,20) IDENT, NPAGE
      NPAGE = NPAGE + 1
      STOP
      E FORMAT (1X,I6,1P10E12.3)
      14 FORMAT (I6,1P8E9.3)
      15 FORMAT (1X,F11.4,11A6,A2)
      16 FORMAT (1X,I11,11A6,A2)
      17 FORMAT (1X)
      18H *****, SNAP S2 CHEMISTRY ***** HARF DEVELOPMENT,
      1
      20 FORMAT (50H1*****, SNAP S2 CHEMISTRY ***** HARF DEVELOPMENT,
      21 FORMAT (10A6,4A5)
      22 FORMAT (1X,A6,1U(3X,A6,3X))
      24 FORMAT (I6,3X,E(1P8E9.3,1H,),3X,A3,I3,I2)
      26 FORMAT (7X,1P6E18.9)
      30 FORMAT (/(1X,30I4))
      34 FORMAT (I4,I2,1X,1P7E10.4)
      35 FORMAT (5X,I4,I2,1X,1F7E12.4)
      END

```

```

C SUBROUTINE COLU1V (HA,CHI,COL,ETA)
C COMPUTES THE INTEGRATED COLUMNAR NUMBER DENSITIES FOR
C COL(1) THE COLUMNAR NUMBER DENSITY FOR O2
C COL(2) THE COLUMNAR NUMBER DENSITY FOR N2
C COL(3) THE COLUMNAR NUMBER DENSITY FOR O3
C ALONG A PATH BEGINNING AT ALTITUDE HA AND EXTENDING TO INFINITY
C AND MAKING AN ANG.-E CHI (RADIANS) WITH RESPECT TO THE LOCAL
C VERTICAL AT HA
C G4I=SOLAR ZENITH ANGLE
C COMMON CONSP(501,25)
C DIMENSION CONC(20),COL(5),TERM(5)
C DATA RE /6371.0/
C DATA A23,A43 / 0.666666666667, 1.333333333333 /
C RHA = RE + HA
C RMIN = RHA*SIN(CHI)
C IF (RMIN .LE. RE) RMIN = RE + 0.0001
C RMINSQ = RMIN*RMIN
C COSC4I = COS(CHI)
C HMIN = ABS(RHA*COSCHI)
C NPT = HA + 1.001
C DO 140 I = 1,4
C TERM(I) = 0.0
C 140 CONTINUE
C ISW = 1
C R1 = RHA + 1.0
C HSUB = HMIN
C IF (COSCHI .GE. 0.0) GO TO 215
C ISW = 0
C LPT = RMIN + 1.0 - RE
C R1 = FLOAT(LPT) + RE
C H1 = SQRT (R1*R1 - RMINSQ)
C HSUB = H1
C R1 = R1 + 1.0
C NA = LPT + 1
C CALL CONCEN(RMIN - RE,CONC,ETA)
C IF (400(NPT-LPT,2) .EQ. 0) GO TO 130
CLMN 10
CLMN 20
CLMN 30
CLMN 40
CLMN 50
CLMN 60
CLMN 70
CLMN 80
CLMN 90
CLMN 100
CLMN 110
CLMN 120
CLMN 130
CLMN 140
CLMN 150
CLMN 160
CLMN 170
CLMN 180
CLMN 190
CLMN 200
CLMN 210
CLMN 220
CLMN 230
CLMN 240
CLMN 250
CLMN 260
CLMN 270
CLMN 280
CLMN 290
CLMN 300
CLMN 310
CLMN 320
CLMN 330
CLMN 340
CLMN 350
CLMN 360

```

```

H13 = H1/3.0
DO 120 I = 1,4
  IF (I .EQ. 3) GO TO 120
  TERM(I) = (2.0*CONSP(I) + CONSP(NA,I))*H13
120  CONTINUE
  NS = LPT + 1
  GO TO 150
130  CONTINUE
  H2 = SQRT(R1*R1 - RMINSQ) - HSUB
  HSUB = HSUB + H2
  R1 = R1 + 1.0
  H12 = 0.5*H1/H2
  H21 = 0.5*H2/H1
  HS3 = (H1 + H2)/3.0
  NB = NA + 1
  DO 140 I = 1,4
    IF (I .EQ. 3) GO TO 140
    YA = CONSP(I)
    YB = CONSP(NA,I)
    YC = CONSP(NB,I)
    TERM(I) = ((YB - YC)*H12 + (YA - YB + YC)*HS3
140  CONTINUE
  NS = LPT + 2
150  CONTINUE
  IF (NS .EQ. NPT) GO TO 205
  NF = NPT - 2
170  CONTINUE
  DO 200 YA = NS, NF, 2
    NB = NA + 1
    NC = NB + 1
    H1 = SQRT(R1*R1 - RMINSQ) - HSUB
    R1 = R1 + 1.0
    HSUB = HSUB + H1
    H2 = SQRT(R1*R1 - RMINSQ) - HSUB
    R1 = R1 + 1.0
    HSUB = HSUB + H2.
    CLMN 370
    CLMN 380
    CLMN 390
    CLMN 400
    CLMN 410
    CLMN 420
    CLMN 430
    CLMN 440
    CLMN 450
    CLMN 450
    CLMN 470
    CLMN 480
    CLMN 490
    CLMN 500
    CLMN 510
    CLMN 520
    CLMN 530
    CLMN 540
    CLMN 550
    CLMN 560
    CLMN 570
    CLMN 580
    CLMN 590
    CLMN 600
    CLMN 610
    CLMN 620
    CLMN 630
    CLMN 640
    CLMN 650
    CLMN 660
    CLMN 670
    CLMN 680
    CLMN 690
    CLMN 700
    CLMN 710
    CLMN 720
  
```

```

H12 = 0.5*H1/H2
H21 = 0.5*H2/H1
HS3 = (H1 + H2)/3.0
DO 180 I = 1,4
  IF (I .EQ. 3) GO TO 180
  YA = CONSP(NA,I)
  YB = CONSP(NB,I)
  YC = CONSP(NC,I)
  TERM(I) = ((YB - YC)*412 + (YB - YA)*H21 + YA + YB + YC)*HS3
  1 + TERM(I)
180  CONTINUE
200  CONTINUE  EQ. 1) 30 TO 220
205  CONTINUE
  ISW = 1
  DO 210 I = 1,4
    TERM(I) = 2.0*TERM(I)
210  CONTINUE
215  CONTINUE
  NS = NPT
  NF = ME*NB*NPT + 30,198 + MOD(NPT,21)
  IF (NPT .GT. 199) GO TO 220
  IF (3*HI .EQ. 0.0) GO TO 250
  GO TO 170
220  CONTINUE
  COL(1) = 1.0E5*TERM(2)
  COL(2) = 1.0E5*TERM(1)
  COL(3) = 1.0E5*TERM(4)
  RETURN
250  CONTINUE
  DO 260 I = 1,4
    TERM(I) = 0.33333333333*CONSP(NPT,I)
260  CONTINUE
  DO 280 NA = NS, NF, 2
    NB = NA + 1
    NC = NB + 1
    CLMN 730
    CLMN 740
    CLMN 750
    CLMN 760
    CLMN 770
    CLMN 780
    CLMN 790
    CLMN 800
    CLMN 810
    CLMN 820
    CLMN 830
    CLMN 840
    CLMN 850
    CLMN 860
    CLMN 870
    CLMN 880
    CLMN 890
    CLMN 900
    CLMN 910
    CLMN 920
    CLMN 930
    CLMN 940
    CLMN 950
    CLMN 960
    CLMN 970
    CLMN 980
    CLMN 990
    CLMN 1000
    CLMN 1010
    CLMN 1020
    CLMN 1030
    CLMN 1040
    CLMN 1050
    CLMN 1060
    CLMN 1070
    CLMN 1080

```

```
CL MN1090
CL MN1100
CL MN1110
CL MN1120
CL MN1130
CL MN1140
CL MN1150

DO 270 I = 1, 4
IF (I .EQ. 3) GO TO 270
TERM(I) = A43*CONSP(N3,I) + A23*CONSP(NC,I) + TERM(I)
270  CONTINUE
280  CONTINUE
      GO TO 220
END
```

SUBROUTINE CONCEN(H, CONC, ETA)

```

SUBROUTINE CONCEN(H,CCNC,ETA)
      PROVIDES AMBIENT CONCENTRATIONS AS A FUNCTION OF ALTITUDE
      CCNC(1) = NO. DENSITY OF N2 IN PARTICLES/CC
      CCNC(2) = NO. DENSITY OF O2 IN PARTICLES/CC
      CCNC(4) = NO. DENSITY OF O IN PARTICLES/CC
      CCNC(7) = NO. DENSITY OF O3 IN PARTICLES/CC

      THIS VERSION (1 MARCH 1971) IS FOR SHAPS2 ONLY.

      COMMON CONSP(501,25)
      DIMENSION CONC(25)
      DATA JMAX /10/
      IF (4 .LE. 200.0) GO TO 115
      DO 110 J = 1, JMAX
      CONC(J) = 0.0
110  CONTINUE
      GO TO 200
115  CONTINUE
      K = 4IN0(200,K)
      HX = H - FLOAT(K - 1)
      DO 130 I = 1, 4
      CX = CONSP(K,I)
      BX = 0.5*(CONSP(I+1,I) - CONSP(I-1,I))
      AX = BX + CONSP(I-1,I) - CX
      CONC(I) = (AX+BX)*HX + CX
      110 CONTINUE
      115 CONTINUE
      RETURN
      END

```

```

SUBROUTINE ROMTST (M,N,DINT,T,RINT,KTEST,EPSS)
C
C   M IS INDEX OF M-TH ENTRY TO ROMTST DURING SINGLE INTERVAL
C   N IS NUMBER OF DIFFERENTIAL EQUATIONS
C   DINT IS VECTOR OF ENDPOINT INTEGRATION VALUES
C   T IS ARRAY IN WHICH ROMBERG EXTRAPOLATION IS COMPUTED
C   RINT IS VECTOR IN WHICH FINAL INTEGRALS ARE RETURNED
C   KTEST IS SET TO 1 IF CONVERGENCE CRITERION IS NOT SATISFIED
C   EPS IS RELATIVE ERROR ALLOWED
C
C   DIMENSION DINT(50)
C   DIMENSION RINT(50)
C   DIMENSION T(50,10)
C
C   IF (M .GT. 1) WRITE (6,6) (DINT(I), I = 1, N)
C   KTEST = 0
C   TIK = 1.0E14
C   DO 150 I = 1, N
C   T(I,4) = 0.0
C   K = 1
C
110  CONTINUE
C   K = K + 1
C   IF (K .GT. M) GO TO 140
C   IF (K .GT. 1) 33 TO 130
C   TA = T(I,1)
C   CA = DINT(I)
C   T(I,1) = CA
C   WA = CA - TA
C   SUM = CA
C   FAC = 1.0
C   GO TO 110
C
130  CONTINUE
C   TA = T(I,K)
C   TA = T(I,K)
C
RTST 10
RTST 20
RTST 30
RTST 40
RTST 50
RTST 60
RTST 70
RTST 80
RTST 90
RTST 100
RTST 110
RTST 120
RTST 130
RTST 140
RTST 150
RTST 160
RTST 170
RTST 180
RTST 190
RTST 200
RTST 210
RTST 220
RTST 230
RTST 240
RTST 250
RTST 260
RTST 270
RTST 280
RTST 290
RTST 300
RTST 310
RTST 320
RTST 330
RTST 340
RTST 350
RTST 360

```

```

FAC = 4.0*FAC
FACB = FAC*T3
DEN = WA/(FACB - CA)
JOV = -ES*VAR(DEN)
IF (JOV .NE. 0) DEN = 0.0
TIK = CA*DEN
T(I,<) = TIK
CA = FACB*DEN
WA = CA - TA
SUM = SUM + TIK
IF (TIK .EQ. 0.0) GO TO 145
GO TO 110
140 CONTINUE
IF (ABS(TIK) .GT. EPS*(1.0E5 + SUM)) KTEST = 1
145 CONTINUE
RINT(I) = SUM
150 CONTINUE
      WRITE(6,7) M,KTEST,(RINT(I), I = 1, N)
      RETURN
C 6 FORMAT (7X,1P6E13.9)
C 7 FORMAT (1X,2I3,1>6E16.9)
END

```

SUBROUTINE SOLLY (OT1-ETA, XALT, TIME, SOLDEC, CHI, ETA)

DATA PI /3.1415926535898/

DATA RE /6.371e0/

PI02 = PI*0.5

T = 1ME

IF (T .GT. 4.32E4) T = T - 8.64E4

XCRIT = ACOS(RE/ (RE + DALT)) + PI02

XMIN = XCRIT-PI/720.0

XMAX = XCRIT+PI/720.0

OLAT = PI02-OTHETA

SINLAT = SIN(OLAT)

COSLAT = COS(OLAT)

SINDEC = SIN(SO-DEC)

COSDEC = COS(SOJEC)

CHI = ACOS(SINLAT*SINDEC+COSLAT*COSDEC+COS(2.*PI*T/86400.))

IF(C4.I.LE.XMIN) GO T0 1

IF (3HI .GE. XMAX) GO T0 2

HDR = (CHI-XMIN)*720.0/PI

ETA = 1.0-(ACOS(1.0-HDR)-(1.0-HDR)*SQRT(2.*HDR-HDR*HDR))/PI

GO T0 3

1 ETA = 1.0

2 ETA = 0.0

3 RETURN

END

SOLL 10
SOLL 20
SOLL 30
SOLL 40
SOLL 50
SOLL 60
SOLL 70
SOLL 80
SOLL 90
SOLL 100
SOLL 110
SOLL 120
SOLL 130
SOLL 140
SOLL 150
SOLL 160
SOLL 170
SOLL 180
SOLL 190
SOLL 200
SOLL 210
SOLL 220
SOLL 230
SOLL 240
SOLL 250

SUBROUTINE SUNPHI(DENSCO,ETA,RATE)
 THIS SUBROUTINE COMPUTES THE PHOTODISSOCIATION RATES AT A
 POINT IN THE ATMOSPHERE DUE TO THE SOLAR FLUX
 DIMENSION PHIZ(30)
 DIMENSION DENSC(10)
 DIMENSION RATE(30)
 DIMENSION FHITOP(30)
 DIMENSION YS(30,10)

```

    DATA PHITOP / 4.59E03,2.62E09,2.86E09,2.00E09,2.59E09,3.30E10,  

    1.35E09,3.10E11,7.97E09,1.44E10,2.28E10,2.07E10,4.05E10,6.96E10,  

    2.1.15E11,2.06E11,5.52E11,1.28E12,2.57E12,5.90E12,1.56E13,3.9E13,  

    3.1.05E14,1.26E14,2.97E14,6.68E14,1.93E15,3.67E15,5.95E15,8.68E15/  

    DATA (XS(I),I=1,30) /1.51E-18,1.03E-18,7.91E-19,5.51E-19,  

    1.6.03E-19,1.13E-18,2.59E-19,1.03E-20,2.91E-19,5.84E-19,3.33E-18,  

    2.1.37E-17,1.40E-17,1.10E-17,6.54E-18,2.96E-18,7.10E-19,2.25E-20,  

    3.1.025E-22,2.50E-23,1.10E-23,7.30E-24,4.12E-24,1.00E-24,6.0.0/  

    DATA (XS(I),I=31,60) /6.0.0,0.1.59E-17,2.29E-17,6.20E-18,  

    1.1.0.23E-17,1.47E-17,6.78E-18,5.16E-18,3.44E-18,1.86E-18,9.36E-19,  

    2.0.22E-19,7.95E-19,6.14E-19,3.87E-19,4.07E-19,1.13E-18,3.88E-18,  

    3.0.82E-18,1.03E-17,5.22E-18,7.35E-19,3.65E-20,1.03E-21,0.0/  

    DATA (XS(I),I=61,90) /7*0.0,1.44E-17,6.0.0,2.65E-18,  

    1.1.4.23E-18,3.80E-18,1.14E-18,6.60E-20,11*0.0/  

    DATA (XS(I),I=91,120) /7*0.0,7.32E-20,6.0.0/  

    1.2.0.6E-19,8.6E-20,2.05E-20,6.7E-21,12*0.0/  

    DATA XS8CH4 /1.50E-17/  

    XS(I,i), ARE MOLECULAR OXYGEN TOTAL CROSS SECTIONS.  

    VALUES FOR I = 1, 30 ARE TAKEN FROM ACKERMAN (1970).  

    VALUES FOR I = 1, 6 WILL BE REVISED LATER  

    XS(I,2) ARE OZONE CROSS SECTIONS FROM ACKERMAN (1970).  

    XS(I,3) ARE WATER VAPOR CROSS SECTIONS.  

    THE ONLY CROSS SECTION USED FOR CH4 IS XS8CH4 AT 1215.7 A.  

    RATE ( 1) IS TOTAL 02 PHOTODISSOCIATION RATE  

    RATE ( 2) IS TOTAL CO2 PHOTODISSOCIATION RATE  

    RATE ( 3) IS TOTAL NO PHOTODISSOCIATION RATE  

    RATE ( 4) IS TOTAL N2O PHOTODISSOCIATION RATE  

    RATE ( 5) IS TOTAL O3 PHOTODISSOCIATION RATE
  
```

C

SPI 10
 SPI 25
 SPI 30
 SPI 40
 SPI 50
 SPI 60
 SPI 70
 SPI 80
 SPI 90
 SPI 100
 SPI 110
 SPI 120
 SPI 130
 SPI 140
 SPI 150
 SPI 160
 SPI 170
 SPI 180
 SPI 190
 SPI 200
 SPI 210
 SPI 220
 SPI 230
 SPI 240
 SPI 250
 SPI 260
 SPI 270
 SPI 280
 SPI 290
 SPI 300
 SPI 310
 SPI 320
 SPI 330
 SPI 340
 SPI 350
 SPI 360

```

C RATE( 6) IS TOTAL H2O PHOTODISSOCIATION RATE
C RATE( 7) IS TOTAL CH4 PHOTODISSOCIATION RATE
C RATE( 8) IS RATE OF O(3P) PRODUCTION FROM O2. PHOTODISSOCIATION
C RATE( 9) IS RATE OF O(1D) PRODUCTION FROM O2. PHOTODISSOCIATION
C RATE(10) IS RATE OF O(3P) PRODUCTION FROM O3. PHOTODISSOCIATION
C RATE(11) IS RATE OF O(1D) PRODUCTION FROM O3. PHOTODISSOCIATION
C FLUX VALUES FOR INTERVALS 1-6 WILL BE REVISED LATER
C INPUT- DENS0(I)=COLUMN NUMBER DENSITY FROM SOURCE TO OBSERVER
C IN PARTICLES PER SQ CM.
C I=1 IS O2, I=2 IS N2 AND I=3 IS O3.
C ETA IS THE FRACTION OF THE SOLAR DISK SHOWING.
C IT COMES FROM SUBROUTINE SOLLY AND RANGES FROM 0 TO 1.
C
C OUTPUT- RATE(I) = REACTION RATES IN REACTIONS PER SEC.
C I=2 IS CO2, I=3 IS NO AND I=4 IS NO2 AT THE OBSERVER.
C RATE(5) IS O3 PHOTODISSOCIATION RATE
C
C SOLAR FLUX AT Z= INFINITY IN PHOTONS PER SQ CM PER SEC. PHITOP(I) SPHI 540
C FOR I=1,30 IS THIS FLUX BROKEN INTO 30 EQUAL WINDOWS OF 0.25 SPHI 550
C RECIPROCAL MICRONS CENTERED AT 9.875 (I=1) TO 2.625 (I=30) SPHI 560
C RECIPROCAL MICRONS. SPHI 570
C
C SET RATES=0 IF ETA=0.
C DO 110 I = 1, 11
C RATE(I) = 0.0
C 110 CONTINUE
C IF (ETA .LE. 0.0) GO TO 500
C
C COMPUTATION OF SOLAR FLUX REACHING HEIGHT Z IN PHOTONS PER SQ CM
C PER SEC. THIS IS THE PORTION OF THE SOLAR FLUX THAT HAS NOT BEEN
C ABSORBED ENROUTE. IT IS MODULATED BY ETA.
C PHIZ(I) FOR I=1,30 ARE THE THIRTY WINDOWS OF THE SOLAR FLUX
C REACHING THE OBSERVER
C COLO2 = ABS(DENS0(1))
C COLO3 = ABS(DENS0(3))
C DO 120 I = 7, 29

```

```

ATTEN = COLO2*XS(I,1) + COLO3*XS(I,2)
PHIZ(I) = ETA*PHITOP(I)*EXP(-ATTEN)
120  CONTINUE
    DJ1 = 0.0
    DO 130 I = 7, 17
        DJ1 = DJ1 + PHIZ(I)*XS(I,1)
130  CONTINUE
    DJ2 = 1.46E-7*ETA/((COLO2*5.71821E-19)**0.793455 + 1.0)
    DO 140 I = 21, 24
        DJ2 = DJ2 + PHIZ(I)*XS(I,1)
140  CONTINUE
    DJ3 = PHIZ(8)*XS(8,2)
    DO 150 I = 18, 27
        DJ3 = DJ3 + PHIZ(I)*XS(I,2)
150  CONTINUE
    DJ4 = PHIZ(28)*XS(28,2) + PHIZ(29)*XS(29,2)
    0.5 = PHIZ(8)*XS(8,3)
    DO 160 I = 15, 13
        DJ5 = DJ5 + PHIZ(I)*XS(I,3)
160  CONTINUE
    DJ6 = PHIZ(8)*XS(8,4)
    DO 170 I = 15, 18
        DJ6 = DJ6 + PHIZ(I)*XS(I,4)
170  CONTINUE
    DJ7 = (PHIZ(7) + PHIZ(8))*1.0E-19
    DO 180 I = 9, 19
        DJ7 = DJ7 + 1.0E-18*PHIZ(I)
180  CONTINUE
    RATE(1) = DJ1 + DJ2
    RATE(2) = DJ6
    RATE(3) = DJ7
    RATE(4) = DJ7
    RATE(5) = DJ3 + DJ4
    RATE(6) = DJ5
    RATE(7) = XS8CH4*PHIZ(8)
    RATE(8) = RATE(1) + DJ2
    SPHI 730
    SPHI 740
    SPHI 750
    SPHI 760
    SPHI 770
    SPHI 780
    SPHI 790
    SPHI 800
    SPHI 810
    SPHI 820
    SPHI 830
    SPHI 840
    SPHI 850
    SPHI 860
    SPHI 870
    SPHI 880
    SPHI 890
    SPHI 900
    SPHI 910
    SPHI 920
    SPHI 930
    SPHI 940
    SPHI 950
    SPHI 960
    SPHI 970
    SPHI 980
    SPHI 990
    SPHI1000
    SPHI1010
    SPHI1020
    SPHI1030
    SPHI1040
    SPHI1050
    SPHI1060
    SPHI1070
    SPHI1080

```

RATE(9) = DJ1
RATE(10) = DJ4
RATE(11) = DJ3
CONTINUE
RETURN
END

SPHI1090
SPHI1100
SPHI1110
SPHI1120
SPHI1130
SPHI1140

```

FUNCTION TKEL (Z)
C RETURNS TEMPERATURES FOR WINTER 30 DEGREE LATITUDE MODEL
C ATMOSPHERE IF Z IS LESS THAN 120 KM, AND APPROXIMATE
C TEMPERATURES FOR HIGH ALTITUDE WINTER MODEL ATMOSPHERE WITH
C EXOSPHERE TEMPERATURE 100K IF Z IS GREATER THAN 120 KM.
C Z IS INPUT ALTITUDE, KM.
C TKEL RETURN VALUE IS ABSOLUTE TEMPERATURE, DEGREES KELVIN.
C LOWER ATMOSPHERE VALUES COMPUTED BY LINEAR INTERPOLATION.
C HIGH ALTITUDE VALUES COMPUTED BY ANALYTICAL APPROXIMATION.
C DIMENSION ZX(15),TX(15)
DATA ZX / 0.000, 2.003, 12.039, 17.069, 18.076, 22.107,
1 32.206, 47.416, 51.484, 59.636, 80.107, 89.361, 101.742,
2 112.096, 120.000 /
DATA TX /288.52, 281.86, 216.15, 203.15, 213.15,
1 233.15, 269.15, 269.15, 253.15, 191.15, 191.03, 22.07,
2 276.22, 334.10 /
IF (Z .GT. 120.0) GO TO 50
DO 10 I = 1, 15
IF (Z - ZX(I)) .LT. 0.0001
10 CONTINUE
20 CONTINUE
TKEL = TX(I)
RETURN
30 CONTINUE
IF (I .GT. 1) GO TO 40
TKEL = 288.52
RETURN
40 CONTINUE
TKEL = TX(I-1) + (TX(I) - TX(I-1)) * (Z - ZX(I-1)) /
1 (ZX(I) - ZX(I-1))
1 RETURN
50 CONTINUE
TKEL = 1000.0 - 665.9*EXP((0.022525*(120.0 - Z)))
RETURN
END

```

```

PROGRAM BCKGND (INPUT,OUTPUT,TAPE5=INPLT,TAPE6=OUTFUT,
  TAPE1,TAPE2)
1  DIMENSION XIO(25,4),XIC(4),FL1(30),STORE(30),IALT(25)
  DIMENSION CATAY(25),COEXT(25),CDEXE(25),NLEVEL(25),NEANC(25)
  DIMENSION LSC(25,10),LCC(25,10),RCM(25,10),RV(25,10),AMASS(25)
  DIMENSION ZANG(7),STAU(7),SRAC(8),RCN(8),RATIO(8)
  DIMENSION LEC(25,20),LBU(25,20),SIR(25,20),SFLLX(25,25),
1 7FLUX(25,25,3)
  DIMENSION CC2(18,2),WATVA(18,2)
  REAL LAMDA
  COMMON /VERCOM/, I, CO2, WATVA, CCEX1, CCEXE
  COMMON /TECCOM/, NLTE
  COMMON /INOLI/, NR, NP, NH
  COMMON/CNC(161,20),TAU(161,20),RAC(161,20),T(161),LAPDA(25),
  1TOTDEN(161)
  DATA (ZANG(I),I=1,7)/0.0,20.0,40.0,60.0,70.0,80.0,90.0/
  DATA (DATATY(I),I=1,25)/8KMETANE,8CAREN D,8FATER VA,8FATRIC
  1,8HNITROUS,8HOZONE PR,8HCZONE NO,18*8H
  NH = 5
  NP = 2.
  NTY = 9
  NW = 0
  PCODE = 1.0
  REWIND 1
  REWIND 2
10  FORMAT(12)  IGAS
  READ(NR,10) IGAS
20  FORMAT(1H,2HNUMBER OF GAS FFCFILES, 13)
  WRITE(NW,26) IGAS
  IGAS=IGAS+1
  EO 170 J=1,IGAS
  ?0  FORMAT(4AE,I3,F7.0)
  READ(NR,30)(XID(J,K), K=1,4), ICH-K,PLIM
  IF (J.EQ.1) GO TO 50
40  FORMAT(7H10 CARD, A6, 20HOUT CF ORDER FOR GAS, 13)
  WRITE(NW,40)(XIC(J,K), K=1,4), J

```

```

50 CO 105 K=1,6
K1=(K-1)*5+1
K2=K1+4
60 FORMAT (5(1H,0,J),E8.1,2X),12,13)
READ(NR,60) (ALT(L),STORE(L),L=K1,K2), ICHK, KCHK
IF (ICHK.EC.0,J) GC TO 80
70 FORMAT (20H,DATA CARD,0UT CF CRCER FCF GAS,13, 3X, 0+CARD NC,, 13)
IFIVE = 5
WRITE (NH,70) J, IFIVE
80 IF (KCHK.EC.0,K) GC TO 90
WRITE (NH,70) J, K
90 DC 100 L=K1,K2
IF (ALT(L).LT.ALTH) GO TO 99
KSET=L
GC TC 120
99 CONTINUE
100 CONTINUE
105 CONTINUE
110 FORMAT (42H,MAX ALT. NOT FOUND CN DATA CARDS - GAS NC,, 13)
WRITE (NH,110) J
120 DO 130 L=1,KSET
130 STCRE(L)=ALCG(STORE(L))
IF (ALTH.GT.150.) GO TC 140
IALT(J)=ALTH-55.
GO TO 150
140 IALT(J)=\$1.0+(ALTH-150.)/5.
150 CALL 1INTERF(ALT,STORE,KSET,1,J)
L1=IALT(J)
DC 160 L=1,L1
160 CONC(L,J)=EXP(CCNC(L,J))
170 CONTINUE
DO 175 J=1,161
175 TCDEN(J)=CCNC(J,IGAS)
READ(NR,30) (XICL(K),K = 1,4), ICHK, KCHK
IF (ICHK.EC.0,1) GC TO 190
180 FORMAT (7H1 CARD, 4A6,26H,CL1 CF CORDER FOR TEMF DATA)

```

```

      WRITE(NW,100) 1X10T(K),K=1,4)
100  CC 245 K=1,6
      K1=(K-1)*5+1
      K2=K1+4
      READ(INR,60)(ALT(L),STORE(L),L=K1,K2), ICHK, KCHK .
      IF(ICHK.EQ.1) GC TO 210
      200  FFORMAT(31HTEMP DATA CARD C01 CF C0DER NC0,12)
      WRITE(NW,210) K
      210  IF(KCHK.EQ.0) GC TO 230
      220  WRITE(NW,200) K
      230  00 240 L=K1,K2
      IF(ALT(L).LT.0.01) GO TO 240
      KSET=L
      GC TC 260
240  CONTINUE
245  CONTINUE
250  FFORMAT(37HMAX AL1. NOT FOUND ON TEMP DATA CARDS)
      WRITE(NW,250)
260  CALL INTERF(ALT,STORE,KSET,2,1)
261  FORMAT(15,EE10.2)
      WRITE(NW,261) (J,(COND(J,I),I=1,IGAS), T(J),J = 1,161)
      IGAS=IGAS-1
      DO 331 I=1,IGAS
      READ(AR,310) TYPE,NLEV ,NBN ,NMAS ,CEXT,DEXB
      310  FFORMAT (A8,22X,12,3X,12,3X,F10.2,4X,2(E12.4,3X))
      DO 311 J=1,25
      IF(TYPE.EQ.CATIATY(J)) GO TO 312
      311  CONTINUE
      WRITE(NW,370)
      370  FFORMAT(36H THE GAS IS NOT LISTED IN THE PROGRAM)
      STCP 1
      312  NSP=J
      NLEVEL(NSP)=NLEV
      NBAND(NSP)=NBN
      AMASS(NSP)=NMAS
      CEXT(NSP)=CEXT
      GC ND1000
      GC ND1010
      GC ND1020
      GC ND1030
      GC ND1040
      GC ND1050
      GC ND1060
      GC ND1070
      GC ND1080

```

```

C CEX8 (NSP) = CEXE
IF (NSP.EC.2) REAC(NR, 320) (CC2(I,1), C02(I,2), I=1,16)
320 FORMAT (6(F5.2,F8.2))
IF (NSP.EC.3) REAC(NR, 321) (ATVA(I,1), VATVA(I,2), I=1,16)
ILEVEL=0
00 313 IJ=1,NLEV
ILEVEL=ILEVEL+1
READ(NR, 330) LSC(NSP, IJ), LOC(NSP, IJ), RCM(NSP, IJ), JGAS,
1JLEVEL
320 FORMAT (2I6,2E12.4,3E8,2I3)
IF (NSP.EC.JGAS) GO TO 314
WRITE(Nh, 340) NSP
340 FORMAT(64HTHE CODE ON THE DATA CCES N1
           : E WITH THE FIRST CARC
           : WHICH IS, IJ)
C STOP 2
314 IF (ILEVEL.EC.JLEVEL) GO TO 313
WRITE(Nh, 350) NSP
350 FORMAT(42H THERE IS A CARD C01 OF SEQUENCE IN GAS AC., I3)
C STCP 3
313 CONTINUE
ILEVEL=0
00 316 IJ=1,NEAN
ILEVEL=ILEVEL+1
READ(NR, 360) LBC(NSP, IJ), LBU(NSP, IJ), STR(NSP, IJ), SFLUX(IJ, NSP),
1(TFLUX(IJ, NSP, J), J=1,3), JGAS, JLEVEL
360 FORMAT (2I6,5E12.4,2I3)
IF (NSP.EC.JGAS) GO TO 322
WRITE(Nh, 340) NSP
STCP 4
322 IF (ILEVEL.EC.JLEVEL) GO TO 316
WRITE(Nh, 350) NSP
C STCP 5
316 CONTINUE
321 CONTINUE
00 900 NLTE = 3, 4
00 850 I = 2, 7
EGND1090
EGND1100
EGND1110
EGND1120
EGND1130
EGND1140
EGND1150
EGND1160
EGND1170
EGND1180
EGND1190
EGND1200
EGND1210
EGND1220
EGND1230
EGND1240
EGND1250
EGND1260
EGND1270
EGND1280
EGND1290
EGND1300
EGND1310
EGND1320
EGND1330
EGND1340
EGND1350
EGND1360
EGND1370
EGND1380
EGND1390
EGND1400
EGND1410
EGND1420
EGND1430
EGND1440

```



```

PHI=ZANG(L)*.017453292
SAVTAU=0.0
STAU(L)=0.0
SRAD(L)=0.0
RANG=0.0
MSET=IAL1(I)
DC 790 M=M1,MSE1
IF (M.GT.91) GO TO 770
D2=M+59+6371
GU TC 780
770 D2=150+(M-51)*546371
780 ANG=ASIN(SIN(PHI)*D1/D2)
DS=SQRT(D1*D1+D2*D2-2.*D1*D2*CCS(PHI-ANG))
DELS=(DS-RANG)*1.0E+15
RANG=0
STAU(L)=STAU(L)+DELS*(1.05*STAU(M,J)+TAU(ih-1,J)))
SAU(L)=SAU(L)+DELS*(0.5*(RAD(M,J)*SM1(MOD(LBU(I,J),10),STAU(L,J))
1+RAD(M-1,J)*SM1(MOD(LBU(I,J),10),SAUTAU)))
SAVTAU=STAU(L)
790 CONTINUE
810 SAVTAU=0.0
STAU(7)=0.0
VRANG=0.0
SRAD(0)=9.0
MSET=IAL1(I)
DO 815 M=K,MSET
MSELS=2*(MSET-K)+1
L=MSET-M+K
IF (L.GT.91) GO TO 811
D2=L+59+6371
GO TO 812
811 D2=150+(L-91)*546371
812 DS=SCRT(D2*D2-01*D1)
D3=D2-6371.
IF (L.LT.MSET) GC TO 813

```

```

RANG=0.5
SA VT1=1.0
GC TC 815
 813 DELS=(RANG-0.5)*1.0E+05
  VRANG = VRANG + DELS
  RANG=0.5
    STAU(7)=STAU(7)+DELS*(0.5*(TAU(L,J)+TAU(L+1,J)))
    SAVT2=SM1(PCD(LEU(I,J),40),S1AU(7))
    SRAD(8)=SRAD(8)+DELS*(0.5*(RAD(L,J)*SAVT2+RAD(L+1,J)*SAVT1)))
    IF (K.GT.1) GC TC 819
    SAVT1=SAVT2
  815 CONTINUE
  M1=K+1
  RANG=0.0
  MSET=IALT(I)
  DO 818 M=M1,MSET
  IF (M.GT.91) GO TO 816
  D2=M+59+6371
  GO TO 817
  816 D2=150+(M-51)*5+6371
  817 DS=SQRT(D2*D2-D1*D1)
  D2=D2-D371
  D3 = D2 - D371
  DELS=(GS-RANG)*1.0E+05
  VRANG = VRANG + DELS
  RANG=0.5
  STAU(7)=STAU(7)+DELS*(0.5*(TAU(M,J)+TAU(M-1,J)))
  SAVT2=SM1(MOD(LEU(I,J),10),S1AU(7))
  SRAD(8)=SRAD(8)+DELS*(0.5*(RAD(M,J)*SAVT2+RAD(M-1,J)*SAVT1)))
  IF (K.GT.1) GO TC 820
  820 SA VT1=SA VT2
  818 CONTINUE
  C 4444  WRITE(NP,4444) HT,SRAD(8),SRAD(1),SRAD(7)
        FFORMAT(FE*1,3E17.4)
        WRITE(NW,740) HT,SRAD(8), HT,(SRAD(M), M= 1,7)
  830 CONTINUE
  840 CONTINUE

```

EGND2530
EGND2540
EGND2550
EGND2560
EGND2570
EGND2580

850 CONTINUE
900 CCNTINUE
REWIND 1
REWIND 2
STOP 77
END

SCERCHIRE-INTERP(ALT,STORE,SET,ACOE,I)
 DIMENSION ALT(30),STORE(30)
 COMMON CCNC(161,10),TAU(161,10),RA0(161,10),T(161),LAPOA(25),
 1TC10EN(161)

```

J=1
A=60.
  60 00 120  K=1,KSET
  10 IF(A-ALT(K))00,20,20
  20 GC TC 30,40,MCCE
  30 CONC(J,I)=STORE(K)
  40 GC TC 50
  40 T(J)=STORE(K)
  50 IF(K.LT.KSET) GC TO 60
  RETURN
  60 IF(J.GE.51) GO TO 70
  61 A=A+1.
  62 GO TO 110
  70 A=A+5.
  70 GC TO 110
  80 FR=(A-ALT(K-1))/(ALT(K)-ALT(K-1))
  80 GC TC 90,100, MODE
  90 CONC(J,I)=STORE(K-1)+FR*STORE(K)-STORE(K-1)
  91 J=J+1
  91 IF(J.GT.51) GC TO 92
  92 A=A+1.
  92 A=A+5.
  92 GC TO 10
  100 T(J)=STORE(K-1)+FR*(STORE(K)-STORE(K-1))
  100 GO TO 91
  110 J=J+1
  120 CONTINUE
  RETURN
  END

```

```

1  SUBROUTINE ERAD (NLEVEL,NEAND,ALIT,TEXCC,VERCC,FM,LSC,LCC,
1    LBC,LBL,EJ,STR,AVE,GONG,SFLUX,TFLUX)
2  C  THIS SECTION COMPUTES FCPUATION OF VIBRATIONAL LEVELS.
3  C  AT PRESENT, TAU IS IGNORED EXCEPT FOR TRANSITIONS TO
4  C  THE GROUND STATE.
5  C
6  DIMENSION EA(10),POWER(10),KL(10)
7  DIMENSION EAHALF(10),TFLUX(10),SFLUX(10)
8  DIMENSION GUP(10),GDOWN(10),GFAC(10)
9  DIMENSION TR2(161),TTH2(161),TOCHN2(161),TTUP2(161)
10  DIMENSION TTH(161,10),TTUP(161,10),TTDCHN(161,10)
11  DIMENSION CONC(161)
12  DIMENSION IVSIG(161),VTSIG(161)
13  DIMENSION VVSIG(161),VDSIG(161)
14  DIMENSION JVNSIG(161),JVRSIG(161)
15  DIMENSION WAVE(250),LSC(250),LCC(250),LEU(250),SIR(250)
16  DIMENSION GNDST(161)
17  DIMENSION CC(18,2),WATVA(18,2)
18  DIMENSION CDEX(25),CDEXB(25)
19  DIMENSION CHEM(161)
20  COMMON /VERCOM/ ICO2,WATVA,CDEX1,CDEXE
21  COMMON /PCFCOM/ VIBPOP(161,10)
22  COMMON/KCEP/KCHEM
23  COMMON/INOLT/ NR,NP,NH
24  EQUIVALENCE (TDOWN2(1),TTDOWN(1,9)),(TTUP2(1),TTUP(1,9))
25  EQUIVALENCE (GNOSTE(1),VIEPOF(1,1))
26  COMMON /TECOM/ NLTE
27  COMMON ZDEN(161,10),BNDTAU(161,10),TEMP(161)
28  COMMON/BNDLAM/ BNDT0(161)
29  AAA = 0.0
30  IF (NLTE .EQ. 4) AAA = 2.0
31  IF (KCHEM .EQ. 1) READ(NR,50) CHEML
32  50  FORMAT (6E12.4)
33  IF (KCHEM .EQ. 1) KCHEM = 0
34  DO 130 N2 = 1, ALIT
35  SUM = 0.0
36  TMP = TEMP(N2)
37  ERAD 10
38  ERAD 20
39  ERAD 30
40  ERAD 40
41  ERAD 50
42  ERAD 60
43  ERAD 70
44  ERAD 80
45  ERAD 90
46  ERAD 100
47  ERAD 110
48  ERAD 120
49  ERAD 130
50  ERAD 140
51  ERAD 150
52  ERAD 160
53  ERAD 170
54  ERAD 180
55  ERAD 190
56  ERAD 200
57  ERAD 210
58  ERAD 220
59  ERAD 230
60  ERAD 240
61  ERAD 250
62  ERAD 260
63  ERAD 270
64  ERAD 280
65  ERAD 290
66  ERAD 300
67  ERAD 310
68  ERAD 320
69  ERAD 330
70  ERAD 340
71  ERAD 350
72  ERAD 360

```

```

DC 110 NL = 2, NLEVEL
JL = (NL - 1)*25 + 1
XYN = YOC(LSC(JL)/10,1)
AP = EXP(-1.43626*WAVE(JL)/10F) * XYN
V18FCF(NZ,NL) = AP
SLM = SLM + AP
110  CCNTINUE
SUM = SLM + 1.6
GNDSTE(NZ) = CONC(NZ)/SUM
CC 120 NL = 2, NLEVEL
V18POP(NZ,NL) = CONC(NZ)*V18FCF(NZ,NL)/SUM
120  CCNTINUE
130  CCNTINUE
DO 135 NL = 2, NLEVEL
JL = (NL - 1)*25 + 1
IF (LCC(JL) * EC. 1) VVWAVE = 2331. - WAVE(JL)
IF (LCC(JL) * EC. 2) VVWAVE = 1556.4 - WAVE(JL)
FAC = 2331.1
IF (LCC(JL) * EC. 2) FAC = 1556.4
135  CCNTINUE
IF (NLTE * EC. 1) GO TO 170
DC 160 NZ = 1, NALT
IF (I * EC. 3) GC TO 136
IF (I * NE. 2) GO TO 145
V1SIG(NZ) = 10.0** (EVAL(CC2(1,1),CC2(1,2),TEMP(NZ)**(-1.0/3.0),E))
VRSIG(NZ) = 10.0** (EVAL(CC2(7,1),CC2(7,2),TEMP(NZ),E))
VNSIG(NZ) = VRSIG(NZ)/EXP(1.43886/TEMP(NZ)*18.0)
VDSIG(NZ) = 10.0** EVAL(CC2(11,1),CC2(11,2),TEMP(NZ)**(-1.0/3.0),E)
1 6)*CENTCF(NZ)
VVUSIG(NZ) = VVDSIG(NZ)*V18FCF(NZ,8)/V18PCF(NZ,5)
GO TO 146
136  CCNTINUE
VNSIG(NZ) = 10.0** (EVAL(HATVF(7,1),HATVA(7,2),TEMP(NZ)
1 4*(-1.0/3.0),E))
VRSIG(NZ) = VNSIG(NZ)*EXP(-1.43879/TEMP(NZ)*736.0)
VTSIG(NZ) = 3.0E-14

```

```

GC TC 15.
140 CONTINUE
VISIG(NZ) = COEXT(I)
VNSIG(NZ) = CCEXB(I)
VRSIG(NZ) = VNSIG(NZ)*EXP(-1.43886/TEMP(NZ)*WAVE)
145 CCNTLNF
TVSIG(NZ) = VISIG(NZ)/GNSTE(NZ)*VIEPOP(NZ,2)
VTSIG(NZ) = VISIG(NZ)*DENTC(NZ)
TVSIG(NZ) = VISIG(NZ)*DENCT(NZ)
TANV = TERF(NZ)
IF (ALTE .LT. 5) GO TO 154
IF (NZ .GT. 41 .AND. NZ .LT. 51) TANV = TEMP(NZ)+FLCAT(NZ-41)
*280.0
146 CONTINUE
FACTCR = EXP(-1.43879*FACTCR)
VNSIG(NZ) = VNSIG(NZ)*DENTC(NZ)*FACTOR/(1.0+FACTCR)
VRSIG(NZ) = VRSIG(NZ)*DENCT(NZ)/(1.0+FACTCR)
147 CONTINUE
148 CONTINUE
WRITE(NF,36)
DO 175 IX = 1, NALT
WRITE(NF,16) (VIBPOP(IX,JX), JX = 1, NLEVEL)
149 CONTINUE
150 CONTINUE
151 CC 180 NE = 1, NEAND
NEX = (NE - 1)*25 + 1
NEC = LEC(NEX)
NI = MOE(NBC/100,110)
NF = MOE(NEC,100)
JI = (NI - 1)*25 + 1
JF = (NF - 1)*25 + 1
KL(NB) = MCL(LEU(NBX)/10,10)
KE(NB) = MCL(LEU(NBX),10)
ENDAN(NE) = 1.0E+4/ (WAVE(JI) - WAVE(JF))
XYR = MOT(LSC(JF)/4.0,11)
XYR = MCC(LSC(IJ)/10,11)
152 ERAD 730
ERAD 740
ERAD 750
ERAD 760
ERAD 770
ERAD 780
ERAD 790
ERAD 790
ERAD 800
ERAD 810
ERAD 820
ERAD 830
ERAD 840
ERAD 850
ERAD 860
ERAD 870
ERAD 880
ERAD 890
ERAD 900
ERAD 910
ERAD 920
ERAD 930
ERAD 940
ERAD 950
ERAD 960
ERAD 970
ERAD 980
ERAD 990
ERAD 1000
ERAD 1010
ERAD 1020
ERAD 1030
ERAD 1040
ERAD 1050
ERAD 1060
ERAD 1070
ERAD 1080

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```

EA(NB) = STR(NEX)*2.804/ENDLAP(NE)*2*XYM
1   *EXP(1.43879*HAVE(JF)/300.0)/XYMM
FCHE(NE) = 1.58065E-20*ENDLAP(NE)
GFAC(NB) = 3.72E-24*STR(NEX)*ENDLAP(NB)**2
1   *EXP(1.43879*HAVE(JF)/300.0)
GUP(NB) = GFAC(NB)*TFLUX(NB)*6.2432
IF (NLTE .LT. 3) GUP(NB) = 0.0
GCOWN(NE) = GFAC(NE)*SFLUX(NE)
IF (NLTE .LT. 4) GDOWN(NE) = 0.0
KEN = KE(NE)
KLN = KL(NB)
ENDL = ENCLAM(NB)
FAC = PCHE(NE)*EA(NB)
SNB = STR(NBX)*EXP(1.43879*HAVE(JF)/300.0)
DC 100 N2 = 1, NALT
ENDTAU(NZ,NE) = TAUHMAX(KLN,KEN,FM,EV,TEMP(NZ),ENDL,SNB,
1   VIEPOP(NZ,NE))
1   IF (NLTE .GT. 1) GO TO 180
ENDRAD(NZ,NE) = VIEPOP(NZ,NE)*FAC
100  CONTINUE
1   IF (NLTE .EQ. 1) GO TO 900
ITER = 0
101  ITER = ITER + 1
NMIN = NALT - 1
DO 190 NE = 1, NMIN
T100W(NALT,NE) = 0.0
TTUF(1,NE) = 0.0
TTH(1,NE) = SIMP(BNCTAU(1,NE),1.0E+5,1)
DO 182 N2 = 2, NMIN
TTH(NZ,NE) = SIMP(ENDTAU(NZ - 1,NE),1.0E+5,2)
102  CONTINUE
CC 104 N2 = 2, NMIN
NY = NALT - NZ + 1
TTUP(NZ,NE) = TTUP(NZ - 1,NE) + TT(NZ - 1,NE)
170CWN(NY,NE) = TTDOWN(NY + 1,NE) + TT(NY,NE)
104  CONTINUE

```

```

TTOCHN(1,NE) = TTDOWN(2,NE) + TT-(1,NE)
TTUP(ALT,AB) = TTUP(NMIN,NE) + TT-(NMIN,NE)
IF (HLTE .GT. 3) GO TO 190
CC 186 NZ = 1, NALT
TTDOWN(NZ,AB) = 0.0
186 CONTINUE
IF (HLTE .GT. 2) GO TO 150
DO 188 NZ = 1, NALT
TTUP(NZ,NE) = 0.0
188 CONTINUE
189 CONTINUE
200 CONTINUE
GC TC(210,220,230,240,250,230,230), I
210 CONTINUE
DC 215 NZ = 1, NALT
VIBPOP(NZ,3) = GNDSTE(NZ)*(GUP(2)*SLM1(KB(2),TTUP(NZ,2))
1 + GDOWN(2)*SLM1(KB(2),TTOCHN(NZ,2))/EA(2) + EA(4))
VIBPUP(NZ,2) = (EA(4) + V1EFOF(NZ,3) + GNDSTE(NZ)
1 *(GUF(1)*SLM1(KB(1),TTUP(NZ,1))
2 + GDOWN(1)*SLM1(KB(1),TTOCHN(NZ,1))
3 + TVSIG(NZ) + 0.75*VNSIG(NZ))
4 /(EA(1) + VTSIG(NZ) + 0.75*VRSIG.
VIBPOP(NZ,4) = GNDSTE(NZ)*(0.25*VNSIG(NZ)
1 + GUP(3)*SLM1(KB(3),TTUP(NZ,2))
2 + GDOWN(3)*SLM1(KB(3),TTOCHN(NZ,3))
3 /(EA(3) + 0.25*VRSIG(NZ))
215 CONTINUE
GC TO 350
220 CONTINUE
NZ = 0
221 NZ = NZ + 1
VIBPCP(NZ,8) = GNDSTE(NZ)*(VNSIG(NZ) + GDCWN(9) + SML1(KB(5)),
1 TDCWN2(NZ) + GUP(5)*SLM1(KB(5),TTUP2(NZ)))
2 / (VRSIG(NZ) + EA(9) + VDOSIG(NZ))
1VS = TVSIG(NZ)
VTS = VTSIG(NZ)

```

```

FCP3 = VIEPOP(NZ,3)
POP4 = VIEPOP(NZ,4)
FCP7 = VIEFCP(NZ,7)
PCP2 = ((TVS + GUP(1)*SLM1(K8(1),T1UP(NZ,1))
8 + 6*2832*GFAC(1)*(XFER(VIEFCP(1,2),TH(1,2),NZ,1)*EA(1))
9 + XFER(VIBFOP(NZ,2),TH(NZ,1),NALT,NZ,2,K8(2))*EA(1))
9 + GDOWN(1)*SM1(K8(1),TTOCH(NZ,1))+GNDTE(N2)
1 + GDOWN(1)*SM1(K8(1),TTOCH(NZ,1))+GNDTE(N2)
1 + FCP3*(EA(2)+VTS)+POP4*(EA(3)+VTS)
2 + POP7*(EA(7)+VTS)/(VTS+EA(1))+VTS;
3 + VIBFOP(NZ,2) = POP2
POP8 = VIEFCP(NZ,8)
POP7 = ((TVS*0.25+GUP(7)*SLM1(K8(7),T1UP(NZ,7))
1 + GDCN(17)*SM1(K8(7),TTOCH(NZ,7))+PCP2
2 + EA(8)*FCP8)/(EA(7)+VTS)
VIBPCF(NZ,7) = POP7
PCP5 = VIEPOP(NZ,5)
POP6 = VIEPOP(NZ,6)
PCP3 = (PCP2*(0.25*TVS+GUP(2)*SLM1(K8(2),T1UP(NZ,2)))
1 + GDOWN(2)*SM1(K8(2),T100W(NZ,2))+POP5*(EA(4)+VTS+TVS)
2/(EA(2)+VTS+TVS)
VIBPOP(NZ,2) = POP3
VIBFCF(NZ,4) = POP4
FCP5 = (PCP3*1.5*TVS+GUP(4)*SLM1(K8(4),T1UP(NZ,4)))
1 + GDOWN(4)*SM1(K8(4),T100W(NZ,4))+POP5*(EA(6)+VTS)
2 + PCP4*(EA(6)+VTS+VTS+VTS)
VIBFCF(NZ,5) = POP5
FCP6 = (FCP4*(0.5*TVS+GUP(6)*SLM1(K8(6),T1UP(NZ,6)))
1 + GDCN(6)*SM1(K8(6),T100W(NZ,6))+POP6
VIBFOP(NZ,6) = POP6
GNDTE(NZ) = CCNC(NZ) - (POP8+POP6+POP5+POP7+FCP4
1 + POP3+FCP2)

```

```

225 IF (NZ.LT.NALT) GO TO 221
      GC TC 350
      CCNTINUE
      1F (ITER * EC, 2) GC TO 40F
      CC 235 NZ = 1, NALT
      VIBFCF(NZ,2) = (TVSIG(NZ) + VVSIG(NZ)
      + GLF(1)*SLM1(KB(1),TTLF(NZ,1))
      1  + 6*2832*GFAC(1)*(XFER(VIEPCF(1,2),TTH(1,1),NZ,1,KB(1))
      2  + XFER(VIEPCP(NZ,2),TTH(NZ,1),NALT,NZ,2,KB(1)) + EP(1)
      3  + GDCWN(1)*SM1(KB(1),TICCN(NZ,1))*GNDSTE(NZ)
      4  + (VTSIG(NZ) + EA(1) + VRSIG(NZ))
      5  CCNTINUE
      225  GO TO 350
      CCNTINUE
      DC 245 NZ = 1, NALT
      VIBFCP(NZ,2) = ((TVSIG(NZ) + VVSIG(NZ)
      1  + GUP(1)*SLM1(KB(1),TTUF(NZ,1))
      2  + 6*2832*GFAC(1)*(XFER(VIBFCF(1,2),TTH(1,1),NZ,1,KB(1))
      3  + XFER(VIBPOP(NZ,2),TTH(NZ,1),NALT,NZ,2,EA(1))
      4  + GDCWN(1)*SM1(KB(1),TTOWN(NZ,1))*GNDSTE(NZ)
      5  + (EA(3) + VTSIG(NZ))*VIEPCF(NZ,3) + AAA*CHEPL(NZ))
      6  / (EA(1) + VTSIG(NZ) + VRSIG(NZ) + TVSIG(NZ))
      VIBPOP(NZ,3) = ((TVSIG(NZ)
      1  + GLF(3)*SLM1(KB(3),TTLP(NZ,3))
      2  + GUP(2)*SLM1(KB(2),TTUF(NZ,2))
      3  + GDCWN(2)*SLM1(KB(2),TLOCN(NZ,2))
      4  + GDCWN(2)*SLM1(KB(3),TICCN(NZ,3))*VIBPCP(NZ,2)
      5  + AAA*CHEPL(NZ))/EA(2) + EA(3) + TVSIG(NZ))
      GNDSTE(NZ) = CCNC(NZ) - VIEPCF(NZ,2) - VRFOP(NZ,3)
      245  CCNTINUE
      250  CCNTINUE
      DC 255 NZ = 1, NALT
      VIBPCF(NZ,6) = GNDSTE(NZ)*(VVSIG(NZ)
      1  + GDCWN(3)*SM1(KB(3),TICCN(NZ,3))
      2  + GUP(3)*SLM1(KB(3),TTUF(NZ,3))
      EFAD2170 EFAD2180
      EFAD2190 EFAD2200
      EFAD2210 EFAD2220
      EFAD2230 EFAD2240
      EFAD2250 EFAD2260
      EFAD2270 EFAD2280
      EFAD2290 EFAD2300
      EFAD2310 EFAD2320
      EFAD2330 EFAD2340
      EFAD2350 EFAD2360
      EFAD2370 EFAD2380
      EFAD2390 EFAD2400
      EFAD2410 EFAD2420
      EFAD2430 EFAD2440
      EFAD2450 EFAD2460
      EFAD2470 EFAD2480
      EFAD2490 EFAD2500
      EFAD2510 EFAD2520

```

```

3 / (VVSIG(NZ) * 1.5 + EA(3))
4 /VIFCF(NZ,5) = (VIBPOP(NZ,6) * VFSIG(NZ) * 0.5
1 + TVSIG(NZ) * VIBPOP(NZ,4) / (V1SIG(NZ) + 5.0 * EA(1))
1 VIFCP(NZ,4) = (VIBPOP(NZ,5) * V1SIG(NZ) + 5.0 * EA(1))
1 + TVSIG(NZ) * VIBPOF(NZ,3)
2 / (TVSIG(NZ) + VTSIG(NZ) + 4.0 * EA(1))
VIFCP(NZ,3) = (VIBPOP(NZ,2) / (TVSIG(NZ) + VTSIG(NZ) + 4.0 * EA(1))
1 + VIFPOF(NZ,7) = (VNSIG(NZ) * VIFFCP(NZ,3)
1 + GNDTE(NZ) * (GUP(2) * SLM1(KB(2),TTUP(NZ,3)
2 + GDOWN(NZ) * SML1(KB(2),TTDWN(NZ,2))) / EA(2)
VIBPOP(NZ,2) = (GNDTE(NZ) * (TVSIG(NZ)
1 + GUP(3) * SLM1(KB(1),TTUP(NZ,1))
2 + GDOWN(NZ,3) * 3.0 * EA(1) + VTSIG(NZ)))
3 + VIBCP(NZ,3) * 3.0 * EA(1) + VTSIG(NZ))
4 / (VTSIG(NZ) + VSSIG(NZ) + EA(1))
755 CONTINUE
350 CONTINUE
DO 360 NE = 1, NBAND
FAC = POWER(NB) * EA(NB)
NBX = (NB - 1) * 25 + 1
NBC = LEC(NBX)
NI = MOD(NB/100,100)
NF = MOD(NBC,100)
KLN = KLN(NB)
KBN = KB(NB)
BNDL = BNCLAM(NB)
JF = (NF - 1) * 25 + 1
SMB = SIR(NBX) * EXP(1.43879 * HAVE(JF) / 300.0)
DO 360 N2 = 1, NALT
BNRAD(NZ,NB) = VIBPOP(NZ,NI) * FAC
IF (NB * EC. 1) GO TO 360
IF (NB * EC. 9) GO TO 360
BNDTAU(NZ,NB) = TAUMAX(KLN, KBN, MP, EV, TEMP(NZ), BNDL, SMB,
1 VIEPOP(NZ,NF))
360 CONTINUE

```

```

4 JN IF :ITER .LT.3) GO TO 181
5 JN CONTINUE
  WRITE (NFE,36)
  DC 850 IX = 1, NALT
  WRITE (NFE,16) (VIBPCF(IX,JX), JX = 1, NLEVEL)
6 JN CONTINUE
  WRITE (NPF,36)
  IF (NLTE .GT. 2)
  C 1  WRITE(NF,8) ((VIBPCF(NZ,NL), NL = 1, 8), NZ = 1, NALT)
  C 1  RETURN
  E FORMAT (8E17.4)
15 FORMAT (1X)
16 FORMAT (3>,10E12.4)
26 FORMAT (6>,718)
36 FORMAT (1F1)
END

```

```

FUNCTION XFER (RAD,TTH,NTCP,NECT,K,K8)
DIMENSION RAD(161),TTH(161),NTCP(161),XFER(161)
NINT = NTCP - NBOT
N1 = NINT/2
KK = MOD(NINT,2)
NPL = NINT + 1
IF (NINT .GT. 0) GO TO 100
XFER = 0.0
RETURN
100 CONTINUE
IF (K .GT. 1) GO TO 200
IF (NINT .GT. 1) GO TO 110
XFER = (0.707107*RAD(2) + SUM2(K8,TTH(1))*RAD(1))*0.5E+5
RETURN
110 CONTINUE
SUM = 0.0
CG 120 NZ = 1, NINT
NY = NINT - NZ + 2
HCLD(NY) = SUM
SUM = SUM + TTH(NY - 1)
120 CONTINUE
HCLD(1) = SUM
DO 130 NZ = 1, NPL
HOLD(NZ) = RAD(NZ)*SUM2(K8,CLC(NZ))
130 CONTINUE
SUM = 0.0
DO 140 N = 1, N8
SUM = SUM + SUM2(HOLD( 2 * N - 1),1.0E+5,3)
140 CONTINUE
IF (KK .EQ. 1) SUM = SUM + SUM2(HCLD(NINT - 1),1.0E+5,2)
XFER = SUM
RETURN
200 CONTINUE
IF (NINT .GT. 1) GO TO 210
XFER = (0.707107*RAD(1) + SUM2(K8,TTH(1))*RAD(2))*0.5E+5
RETURN

```

```

21n  CONTINUE
      SUM = 0.0
      DC 220 NZ = 1, NPL
      HCLD(NZ) = SUM
      SUM = SLM + TTR(NZ)
22n  CONTINUE
      DC 230 NZ = 1, NPL
      HOLE(NZ) = RAO(NZ)*SDN2(KE, TLD(NZ))
23n  CONTINUE
      SUM = 0.0
      DC 240 N = 1, N
      SLM = SLM + SIMP(HCLD( 2* N - 1), 1.0E+5, 3)
24n  CONTINUE
      IF (KK .EQ. 1)  SUM = SUM + SIMP(HCLD(NINT - 1), 1.0E+5, 2)
      XFER = SUM
      RETURN
      END

```

```

FUNCTION EVAL (XP,YP,X,N).
DIMENSION XF(N),YP(N)
H = XP(2) - XP(1)
IF (X .GE. XP(N - 1)) GO TO 120
I = 1
110 CONTINUE
I = I + 1
IF (X .GE. XP(I + 1)) GO TO 110
GO TO 130
120 CONTINUE
I = N - 1
130 CONTINUE
XH = (X - XP(I))/H
C = YF(I)
B = 0.5*(YP(I + 1) - YP(I - 1))
A = 0.5*(YP(I - 1) - C - C + YP(I + 1))
EVAL = (A*XH + B)*XH + C
RETURN
END

```

```
FUNCTION TAUMAX (KL,KE,RM,EV,T,FLAM,S,DEN)
SIG = 1.43879*EV/T
TAUMAX = 5.3613E-18*SQRT(RM/T)*FLAM*DEN*S*SIGMAX(KL,KE,SIG)
RETURN
END
```

1MAX 10
1PAX 20
1MAX 30
1MAX 40
1MAX 50

FUNCTION SUMAX (KL, KB, SIG)
C SUMAX COMPUTES THE RELATIVE STRENGTH OF THE STRONGEST LINE
C IF KE = 1, SIGMA-SIGMA TRANSITION
C IF KB = 2, SIGMA-PI TRANSITION

GO TC (110, 120, 130), KB
CONTINUE
110 TJM = 0.5 * (SQR1(0.25 + 2.0/SIG) - 1.0)
A = 0.5 * (1JM + TJM + 1.0)
GO TO 200
120 CONTINUE
TJM = 0.5 * (SQR1(2.0/SIG) - 1.0)
A = TJM + 1.0
GC TO 200
130 CONTINUE
SMAX = 1.0
RETURN
200 CONTINUE
TJM = A * EXP(-SIG*TJM*(TJM + 1.0))
SMAX = SJM / CJPART (KL, SIG)
RETURN
END

```
FUNCTION SINT (A,B,C,H,K)
IF (K .GT. 1)  GO TO 110
SINT = (B .R*8 + 5.0*A - C)*H/12.0
RETURN
CONTINUE
SINT = (B .R*8 + 5.0*C - A)*H/12.0
RETURN
END
110
```

```

FUNCTION CJPART (K,SIG)
C   CJPART COMPUTES THE ROTATIONAL PARTITION FUNCTION FCR A
C   ROTATIONAL, SIG * LE. 0.2*
C   K = 1, ALL LEVELS POPULATED
C   K = 2, EVEN LEVELS POPULATED
C   K = 3, ODD LEVELS POPULATED
C
C   IF (SIG .GT. 0.2) STOP
C   X = SIG
C   IF (K - 2) 110,120,130
C   COEFFICIENTS ARE FROM RLM DALTE-EV
C 110  CONTINUE
C   CJPART = (((((0.00386500232857*SIG + 0.012571835471)*X
C   1 + 0.0666756164530)*X + 0.333333133379)*X + 1.00603000017)/SIG
C   RETURN
C 120  CONTINUE
C   CJPART = (((((62.5879214193*SIG - 29.5697177693)*SIG
C   1 + 5.4969267096)*SIG - 0.502572235608)*SIG
C   2 + 0.025737819346)*SIG + 0.0326250901506)*SIG
C   3 + 0.166670220770)*SIG + 0.45555559456)/SIG
C   RETURN
C 130  CONTINUE
C   CJPART = (((((29.5703117876 - 62.56/4596502*SIG)*SIG
C   1 - 5.49573273669)*SIG + 0.565750542701)*SIG
C   2 - 0.0170297551676)*SIG + 0.0328315889069)*SIG
C   3 + 0.166663112387)*SIG + 5.00000544)/SIG
C   RETURN
C   END
C
CJPART 10
CJFR 20
CJPR 30
CJPR 40
CJPR 50
CJPR 60
CJPR 70
CJPR 80
CJPR 90
CJPR 100
CJPR 110
CJPR 120
CJPR 130
CJPR 140
CJPR 150
CJPR 160
CJPR 170
CJPR 180
CJPR 190
CJPR 200
CJPR 210
CJPR 220
CJPR 230
CJPR 240
CJPR 250
CJPR 260
CJPR 270

```

```

FUNCTION SIMP (A,H,K)
DIMENSION A(3)
IF (K - 2) 100,110,120
100  CCNTINUE
      SIMP = (8.0*A(2) + 5.0*A(1) - A(3))*H/12.0
      RETURN
110  CCNTINUE
      SIMP = (8.0*A(2) + 5.0*A(3) - A(1))*H/12.0
      RETURN
120  CCNTINUE
      SIMP = (4.0*A(2) + A(1) + A(3))*H/3.0
      RETURN
      END

```

```

FUNCTION SP1 (K,TAU)
T = ABS(TAU)
IF (T .EQ. 0.0) GO TO 300
IF (K .GE. 2) GO TO 200
IF (T .GT. 4.0) GO TO 110
X = (T - 2.0)*5
SP1 = (((((2.35491E-03)*X - 8.90535E-03)*X + 2.56223E-02)*X
1 - 7.07877E-02)*X + 1.63735E-01)*X - 3.01749E-01)*X + 0.426845
1 RETURN
110 CONTINUE
IF (T .GT. 10.0) GO TO 120
X = (T - 7.0)/3.0
SP1 = (((((5.52297E-04)*X - 1.79043E-03)*X + 4.05109E-03)*X
1 - 1.04749E-02)*X + 2.59109E-02)*X - 6.01708E-12)*X + 0.134123
1 RETURN
120 CONTINUE
IF (T .GT. 100.0) GO TO 130
Y = ALOC(1)
X = 9.210340371976/Y - 3.0
SP1 = (((((-6.24516E-04)*X - 6.79378E-04)*X + 6.98590E-03)*X
1 - 1.28150E-03)*X - 6.31784E-03)*X + 3.78904E-02)*X
2 + 8.90441E-01)/T
1 RETURN
130 CONTINUE
Y = ALOC(1)
X = 9.210340371976/Y - 1.0
SP1 = (((((6.12738E-04)*X - 2.93434E-04)*X - 4.36163E-04)*X
1 + 1.35027E-02)*X - 3.80088E-04)*X + 3.23441E-02)*X
2 + 8.17407E-01)/T
1 RETURN
139 CONTINUE
IF (T .GT. 4.0) GO TO 210
X = (T - 2.0)*5
SP1 = (((((1.36071E-03)*X - 5.29504E-03)*X + 1.56249E-02)*X
1 - 4.074039E-02)*X + 1.026175E-01)*X - 2.086333E-01)*X + 3.517573
1 RETURN
200 CONTINUE
IF (T .GT. 4.0) GO TO 210
X = (T - 2.0)*5
SP1 = (((((1.36071E-03)*X - 5.29504E-03)*X + 1.56249E-02)*X
1 - 4.074039E-02)*X + 1.026175E-01)*X - 2.086333E-01)*X + 3.517573
1 RETURN

```

```

210  CONTINUE
    IF (T .GT. 10.0)  GC TO 220
    X = (T - 7.0) / 3.0
    SM1 = (((((13.764211E-04*X - 1.025384E-03)*X + 3.041166E-03)*X
    1  " 1.05360E-02)*X + 3.07476E-02)*X - 8.14775E-02)*X + 0.1541308
    1  RETURN
220  CONTINUE
    1F (T .GT. 100.0)  GO TO 230
    Y = ALOG(T)
    X = 9.0210240371976/Y - 3.0
    SM1 = ((((-7.53415E-03*X - 8.087124E-03)*X + 6.62199E-02)*X
    1  + 1.0304245)/T
    1  RETURN
230  CONTINUE
    Y = ALOG(T)
    X = 9.0210240371976/Y - 1.0
    SM1 = (((((12.55067E-03 - 5.82519E-04*X)*X + 1.055669E-03)*X
    1  + 1.021174E-03)*X + 4.076165E-02)*X + 1.018445)/T
    1  RETURN
240  CONTINUE
    SM1 = 1.0
    RETURN
    END

```

```

FUNCTION SLM1 (K,TAU)
T = ABS(TAU)
IF (T .EQ. 0.0) GO TO 300
IF (K .EQ. 1) GO TO 200
IF (T .EQ. 1.0) GO TO 110
X = (T - 0.5) * 2.0
SLM1 = (((((2.30089E-03*X - 2.29897E-03)*X - 2.19020E-02)*X
1 + 8.432313E-04)*X + 4.56944E-03)*X - 1.03180E-02)*X
2 + 3.26304E-02)*X - 1.15722E-01)*X + 3.34592E-01
RETURN
110 CONTINUE
IF (T .EQ. 4.0) GO TO 120
X = (T - 2.5) / 1.5
SLM1 = (((((9.76236E-04 - 3.52846E-04*X - 1.79436E-03)*X
1 + 4.96516E-03)*X - 1.33950E-02)*X + 3.19120E-02)*X
2 - 6.75970E-02)*X + 1.23984E-01
RETURN
120 CONTINUE
IF (T .EQ. 10.0) GO TO 130
X = (T - 7.0) / 3.0
SLM1 = (((((3.17194E-04*X - 2.05675E-04)*X + 1.48227E-03)*X
1 - 3.59295E-03)*X + 8.66454E-03)*X - 1.97823E-02)*X + 1.0439983
RETURN
130 CONTINUE
IF (T .EQ. 100.0) GO TO 140
Y = ALOC(1)
X = 9.210240371976/Y - 3.0
SLM1 = (((((3.77202E-04*X - 6.03531E-04)*X - 1.17101E-03)*X
1 + 1.10506E-02)*X + 0.293204)/1
RETURN
140 CONTINUE
Y = ALOC(1)
X = 9.210240371976/Y - 1.0
SLM1 = (((((9.45179E-05*X + 2.68993E-04)*X - 5.46678E-04)*X
1 + 1.01193E-02)*X + 0.272108)/1
RETURN

```

```

200  CONTINUE
    IF (T .GT. 1.0) GO TO 210
    X = (T - 0.5)*2.0
    SLM1 = (((((1.53668E-03*X - 1.53539E-03)*X - 1.46271E-03)*X
    1 + 5.61827E-04)*X + 3.06453E-03)*X - 7.08252E-03)*X
    2 + 2.42681E-02)*X - 9.93037E-02)*X + 3.65233E-01
    RETURN
210  CONTINUE
    IF (T .GT. 4.0) GO TO 220
    X = (T - 2.5)/1.5
    SLM1 = (((((6.0062E-04*X - 1.73522E-03)*X + 3.65978E-03)*X
    1 - 1.05347E-02)*X + 2.95629E-02)*X - 7.50205E-02)*X + 0.16410E
    RETURN
220  CONTINUE
    IF (T .GT. 10.0) GO TO 230
    X = (T - 7.0)/3.0
    SLM1 = (((((2.55944E-04*X - 7.10512E-04)*X + 1.57111E-03)*X
    1 - 4.31080E-03)*X + 1.14462E-02)*X - 2.80911E-02)*X + 0.0643049
    RETURN
230  CONTINUE
    IF (T .GT. 100.0) GO TO 240
    Y = ALOG(T)
    X = 9.210340371576/Y - 3.0
    SLM1 = ((((-1.51727E-03*X - 1.40803E-03)*X + 1.089331E-02)*X
    1 + 0.428568)/1
    RETURN
240  CONTINUE
    Y = ALOG(T)
    X = 9.21034037976/Y - 1.0
    SLM1 = (((6.45913E-04*X + 2.46757E-04)*X - 1.12575E-04)*X
    1 + 1.40752E-02)*X + 0.394276)/1
    RETURN
300  CONTINUE
    SLM1 = 0.5
    RETURN
    END

```

```

FUNCTION SCM2 (K,TAU)
T = ABS(TAU)
IF (T .EQ. 0.0) GO TO 300
IF (K .GT. 1) GO TO 200
IF (T .GT. 1.0) GO TO 110
X = (T - C.5)*2.0
SDM2 = (((((1.96434E-01)*X-1.37918E-01)*X-5.44871E-01)*X
1 + 3.48950E-01)*X+5.84914E-01)*X-3.35128E-01)*X-2.0.57842E-01)*X
2 + 1.44634E-01)*X+7.67977E-02)*X-3.36629E-02)*X+3.0.83636E-03)*X
3 - 6.16125E-02)*X-2.74611E-01)*X+5.26563E-01+T*ALOG(T)/SGRT(3.)
RETURN
110 CONTINUE
IF (T .GT. 4.0) GO TO 120
X = (T - 2.5)/1.5
SDM2 = (((((1.6.71928E-04*X-1.34115E-03)*X+1.38025E-03)*X
1 - 3.42908E-03)*X+5.3267E-03)*X-1.95584E-02)*X+3.76565E-02)*X
2 - 5.98765E-02)*X+6.35365E-02
RETURN
120 CONTINUE
IF (T .GT. 10.0) GO TO 130
X = (T - 7.0)/3.0
SDM2 = (((((1.6.91884E-05*X-1.72263E-04)*X+2.79078E-04)*X
1 - 6.2767E-04)*X+1.45592E-03)*X-2.56094E-03)*X+5.21475E-03)*X
2 - 6.13190E-03)*X+9.28992E-03
RETURN
130 CONTINUE
IF (T .GT. 100.0) GO TO 147
Y = ALOG(1)
X = 9.0.210340371976/Y - 3.0
SDM2 = ((((-1.78966E-04*X-1.12080E-03)*X+2.02868E-03)*X
1 + 3.42340E-04)*X-5.16189E-03)*X+2.21993E-02)*X+4.28605E-01
SCM2 = SCM2/(T+T)
RETURN
147 CCNTINUE
Y = ALOG(1)
X = 9.0.210340371976/Y - 1.0

```

```

SDM2=(6.3*3204E-04*x+6.11261E-04)*x+5.05934E-04)*x+1.71698E-02)*x
2+3.05175E-01 SDM2=SDM2/(T*T)
RETURN
200 CONTINUE
IF (T .GT. 1.0) GC TC 210
X = (T - 0.5)*2.0
SDM2={(((((-5.54556E-01*x+3.82958E-01)*x+1.68014E+00)*x
1-1.06922E+00)*x-2.0*x213E+0)*x+1.15274E+00)*x+1.17482E+00)*x
2-5.09857E-01)*x-3.55692E-01)*x+1.54264E-01)*x+4.0*x3668E-02)*x
3+1.06675E-03)*x-7.54472E-02)*x-2.65402E-01)*x+5.61024E-01
4+T*ALCG(1)/SQR(T)*())
RETURN
210 CONTINUE
IF (T .GT. 4.0) GO TO 220
X = (T - 2.5)/1.5
SDM2={(((5.78273E-04*x-1.15017E-03)*x+1.95966E-02)*x
1-3.00744E-03)*x+8.15919E-03)*x-1.0*x4944E-02)*x+3.0*x4034E-02)*x
2-7.0*x15164E-02)*x+9.0*x8052E-02
RETURN
220 CONTINUE
IF (T .GT. 10.0) GO TO 230
X = (T - 7.0)/3.0
SDM2={((((-1.58499E-04*x+3.08493E-04)*x-6.0*x423E-04)*x
1+3.0*x5552E-03)*x-3.0*x1034E-03)*x+7.0*x9235E-03)*x-1.0*x493E-02)*x
2+1.0*x7007E-02
RETURN
230 CONTINUE
IF (T .GT. 100.0) GO TO 240
Y = ALOG(T)
X = 9.0*210340371976/Y - 3.0
SDM2={((1.127664E-04*x-2.05836E-04)*x-8.0*x55043E-03)*x-1.0*x7621E-02)
1+5.0*x6025E-02)*x+2.0*x072E-01
SUM2 = SDM2/(1*T)
RETURN
240 CONTINUE

```

```
Y = ALUG(1)
X = 9.21034037576/Y - 1.0
SDM2=6(((1.19945E-03*X-3.60578E-04)*X-1.48588E-05)*X
1.41*81041E-03)*X+3.40447E-03)*X+2.26935E-02)*X+7.19045E-01
SDM2 = SDM2/(T*T)
RETURN
300 3CONTINUE
      SDM2=1./SGRT(2.)
      RETURN
      END
```

```

PROGRAM SPECTRA (XDATA,OLTPUT,TAPE1=XCATA,TAPE2=OLTFLT,TAPE4)
DIMENSION LSC(10),LSC(110),RCM(110),EV(10),LEC(10),LCL(10),SF(10)
DIMENSION P(100),Q(100),R(100),FS(100),QS(100),RS(100)
DIMENSION HCLAM(450),HCLAM(450),HCLSE(450),HRAC(600)
DIMENSION ROTLAM(250),RCTEA(250),ROTLSE(250),RCTST(250)
DIMENSION AVLAM(200)
DIMENSION CCN(161,10),TEMF(161),FRCC(161)
DIMENSION AVTEMP(12,10),EVTEMP(12,10)
DIMENSION CCLCAT(12,10),CRCAT(12,10)
DIMENSION CR(40)
DIMENSION CRH(40)
DIMENSION ENU(250),ENL(250),ENERGY(250)
DIMENSION KVLTR(450),EA(250)
DIMENSION TAU(250),RAD(250)
DIMENSION RADA(50),RADE(50),RAAC(50)
DIMENSION EALC(250),EALR(250)
DIMENSION SPEC(201,12),SPECCE(201,12),SPECCC(201,12)
DIMENSION EAMOL(10)
EQUivalence (P(1),HFAC(1)),(C(1),HRAC(101)),(R(1),HRAC(201)),
1 (S(1),HRAD(301)),(GS(1),HRAC(401)),(RS(1),HRAD(501))
CCMHCN SPECAC, SPECB, SPEC
CCMHCN /HCCOM/ HHOLAM, HCCSTR, HCLSE, HRAD
CCMHCN /RCTCOM/ ROTLAM, ROTEA, ROTLSE, ROTST
REWIND 4
NCUT = 0
NLN = 100
NLT = 61
CALL ROTATE
DO 590 NCASES = 1, 2
  WRITE (2,16)
  BLAM = 5.0
  DO 105 I = 1, 201
    AVLAM(I) = BLAM
    BLAM = BLAM + 0.1
    DO 105 J = 1, 12
      SPECAC(I,J) = 0.0
      SPECAC(I,J) = 1.0
      SFTR 10
      SFTR 20
      SFTR 30
      SFTR 40
      SFTR 50
      SFTR 60
      SFTR 70
      SFTR 80
      SFTR 90
      SFTR 100
      SFTR 110
      SFTR 120
      SFTR 130
      SFTR 140
      SFTR 150
      SFTR 160
      SFTR 170
      SFTR 180
      SFTR 190
      SFTR 200
      SFTR 210
      SFTR 220
      SFTR 230
      SFTR 240
      SFTR 250
      SFTR 260
      SFTR 270
      SFTR 280
      SFTR 290
      SFTR 300
      SFTR 310
      SFTR 320
      SFTR 330
      SFTR 340
      SFTR 350
      SFTR 360
  105
  590

```

```

SPECB(I,J) = 0.0
105  CONTINUE
DC 110 I = 1, NALT
    IF (I .LT. 21) TEMP(I) = 255.0 - (I - 1)*3.7
    IF (I .LT. 20) TEMP(I) = 181.0
    IF (I .LT. 31) TEMP(I) = 181.0 + (I - 31)*2.5
    IF (I .LT. 41) TEMP(I) = 210.0 + (I - 41)*4.7
    IF (I .LT. 51) TEMP(I) = 257.0 + (I - 51)*9.2
110  CONTINUE
    WRITE (2,8) TEMP(I), I = 1, NALT
    WRITE (2,14)
    READ (1,6) NSPTOT
    DO 400 NSP = 1, NSPTOT
        READ (1,6) ISP
        READ (1,41) NLEVEL, NBAND, RM
        DO 210 I = 1, NLEVEL
        READ (1,41) LSC(I), ECC(I), RCP(I), EV(I)
        210  CONTINUE
        DO 220 I = 1, NEAND
        READ (1,41) LBC(I), LBU(I), STR(I)
        220  CONTINUE
        READ (1,6) NALT, NREL
        READ (1,42) ((CON(NZ,NL), NL = 1, 8), NZ = 1, NALT)
        COMPUTE MEAN TEMPERATURES AND CGLMN COUNTS
        K = 12
        DC 129 NL = 1, NLEVEL
        DO 112 I = 1, 61
        PROD(I) = CON(I,NL)*TEMP(I)
        112  CONTINUE
        TF = 0.0
        TC = 0.0
        NA = 61
        DO 120 I = 1, K
        TF = TF + SIMP (PROD(NA - I), 1.0E+5, 2)
1        + SIMP (PROD(NA - 3), 1.0E+5, 3) + SIMP (PROD(NA - 5), 1.0E+5, 3)
120

```

```

TC = TC + SIMP(CCN(NA - 2,NL),1.0E+5,2)           SFTR 730
1 + SIMP(CCN(NA - 3,NL),3.0E+5,3) + SIMP(CCN(NA - 5,AL),1.0E+5,3) SFTR 740
COLCNT(K - I + 1,NL) = TC                           SFTR 750
AVTEMP(K - I + 1,NL) = TP/TC                         SFTR 760
NA = NA - 5                                         SFTR 770
HCRCNT(I,NL) = 0.0                                   SFTR 780
SPTR 790
SPTR 800
SPTR 810
SPTR 820
SPTR 830
SPTR 840
SPTR 850
SPTR 860
SPTR 870
SPTR 880
SPTR 890
SPTR 900
SPTR 910
SPTR 920
SPTR 930
SPTR 940
SPTR 950
SPTR 960
SPTR 970
SPTR 980
SPTR 990
SPTR 1000
SPTR 1010
SPTR 1020
SPTR 1030
SPTR 1040
SPTR 1050
SPTR 1060
SPTR 1070
SPTR 1080

120  CCNTINUE
      WRITE (2,6) (COLCNT(I,NL), I = i, K)
      WRITE (2,14) (AVTEMP(I,NL), I = 1, K)
      WRITE (2,14)
      REASE = 6.431E+8
DO 120 I = 1, K
      TPH = 0.0
      TCH = 0.0
      NA = 61
      RE2 = REASE*REASE
      RTOP = 6.431E+8 + NALT*1.0E+5
      SVH = SCR1(RTOP*RTOP - RE2)
      KK = K - I + 1
DO 125 J = 1, KK
      RTOP = RTCP - 1.0E+5
      STH = SCR1(RTOP*RTOP - RE2)
      H5 = SVF - STH
      SVH = STH
      RTOP = RTCP - 1.0E+5
      STH = SCR1(RTOP*RTOP - RE2)
      H4 = SVF - STH
      SVH = STH
      RTOP = RTCP - 1.0E+5
      STH = SCR1(RTOP*RTOP - RE2)
      H3 = SVF - STH
      SVH = STH
      RTOP = RTCP - 1.0E+5
      STH = SCR1(RTOP*RTOP - RE2)
      H2 = SVH - STH

```

```

SVH = STH
RTCP = RTCF " 1.0E+5
STH = SCR1CABS(RTOP*RTOF - RE2)
H1 = SVH - STH
SVH = STH
TPH = TPH + QINT( PROD(NA - 2), T4, H5, 2)
1 + QINT( PFCD(NA - 3), H3, T4, 3) + CINT( PROD(NA - 5), T1, H2, 3)
TCH = TCH + CINT( CON(NA - 2, NL), T4, H5, 2)
1 + QINT( CON(NA - 3, NL), H3, H4, 3) + CINT( CON(NA - 5, NL), H1, T2, 3)
NA = NA - 5
125 CONTINUE
HORCNT(I, NL) = TCH
EVTEMP(I, NL) = TPH/TCH
RBASE = REASE + 5.0E+5
126 CNTINUE
WRITE(2,6) (HRCNT(I, NL), I = 1, K)
WRITE(2,14)
WRITE(2,8) (EVTEMP(I, NL), I = 1, K)
WRITE(2,14)
127 CNTINUE
00 400 NE = 1, ABAND
00 230 I = 1, NRLEV
READ(1,43) HT, RADC(I), RADC(I), RACH(I)
128 CNTINUE
NEC = LEC(NB)
NI = MOD(NEC/100,100)
NF = MOD(NEC,100)
CENTER = RCM(NI) - RCM(NF);
SAB = STR(NB)*EXP(1.43879*RCM(NF)/307.0)
KL = MOD(LEU(NE)/10,10)
KB = MOD(LEU(NE),10)
1F (ISP * EC. 3) GO TO 260
1F (ISP * EC. 6) GO TO 260
1F (ISP * EC. 7) GO TO 260
CALL RCTPCS (CENTER, BV(NI), EV(NF), F, Q, R, 1)
CC 250 I = 1, 1E

```

```

CALL ROT1R (RADA(I),RM,EV(NF),AVTEMP(I,NF),COLCNT(I,NF)),
1 SNE,PS,GS,RS,KE,1,P,Q,R)
CALL FILTER (SPEC(I,I),FS,P,RLN)
CALL FILTER (SPEC(I,I),GS,C,RLN)
CALL FILTER (SPEC(I,I),RS,R,RLN)
CALL RC1S1R (RADC(I),RM,EV(NF),BVTEMP(I,NF),HRCNT(I,NF)),
1 SNE,FS,GS,RS,KB,1,P,G,R)
CALL FILTER (SPECB(I,I),PS,F,RLN)
CALL FILTER (SPECB(I,I),GS,C,RLN)
CALL FILTER (SPECB(I,I),RS,R,RLN)
CALL ROT1R (RADC(I),RM,EV(NF),BVTEMP(I,NF),2.0*HRCNT(I,NF)),
1 SNE,FS,GS,RS,KP,1,P,Q,R)
CALL FILTER (SPEC(I,I),PS,F,RLN)
CALL FILTER (SPEC(I,I),GS,C,RLN)
CALL FILTER (SPEC(I,I),RS,R,RLN)
CONTINUE
GC TC 260
260 CONTINUE
DC 270 I = 1, 12
IF (ISP .AE. 3) GO TO 265
CALL WA1S1R (RADA(I),RM,AVTEMP(I,NF),COLCNT(I,NF),1)
CALL FILTER (SPEC(I,I),HRAD,RC1LAM,250)
CALL WA1S1R (RADA(I),RM,AVTEMP(I,NF),COLCNT(I,NF),2)
CALL FILTER (SPEC(I,I),HRAD,RC1LAM,434)
CALL WA1S1R (RADA(I),RM,AVTEMP(I,NF),HRCNT(I,NF),1)
CALL FILTER (SPEC(I,I),HRAD,RC1LAM,250)
CALL WA1S1R (RADA(I),RM,AVTEMP(I,NF),HRCNT(I,NF),2)
CALL FILTER (SPEC(I,I),HRAD,RC1LAM,434)
CALL WA1S1R (RADC(I),RM,AVTEMP(I,NF),2.0*HRCNT(I,NF),1)
CALL FILTER (SPEC(I,I),HRAD,RC1LAM,250)
CALL WA1S1R (RADC(I),RM,AVTEMP(I,NF),2.0*HRCNT(I,NF),2)
CALL FILTER (SPEC(I,I),HRAD,RC1LAM,434)
GO TO 270
CONTINUE
265 CALL WA1S1R (RADA(I),RM,AVTEMP(I,NF),COLCNT(I,NF),3)
CALL FILTER (SPEC(I,I),HRAD,PS,2)

```



```
REWIND 4
STOP
4  FORMAT (21F 10.3)  ERROR IN AECUE CAF(E)
6  FORMAT (61F1)
8  FORMAT (6E12.4)
11  FORMAT (6I3,F12.6,3F9.2,F5.1,E12.3,F12.3)
12  FORMAT (4F12.4,E12.4,F12.6)
14  FORMAT (1)
16  FORMAT (1)
18  FORMAT (3X,F8.2,12E10.3)
41  FORMAT (216,5E12.4)
42  FORMAT (8E10.4)
43  FORMAT (F6.1,3E17.4)
END
```

```
SFTIR 10
SFTIR 20
SFTIR 30
SFTIR 40
SFTIR 50
SFTIR 60
SFTIR 70
SFTIR 80
SFTIR 90
SFTIR 100
SFTIR 110
SFTIR 120
SFTIR 130
SFTIR 140
```

```

SUBROUTINE WATSTR (RA0, RM, T, CEN, N)
DIMENSION HNOLAM(450), HHCSTR(450), HCOLSE(450), HRAC(600)
DIMENSION KOTLAM(250), RCTEA(250), RCTLSE(250), RCTS1(250)
DIMENSION STR03(32), ENLC3(32), NLC3(32)
DATA STR03 / 0.160, 0.306, 0.476, 0.857, 1.242, 1.693, 1.925, 1.693,
1 1.564, 1.244, 1.822, 2.057, 1.911, 1.133, 0.0337, 0.0067, 0.0040, 0.0044, 0.0044,
2 0.0047, 0.0051, 0.0042, 0.0038, 0.0036, 0.0096, 0.0066, 0.0066, 0.0066, 0.0066,
3 0.0068, 0.0064, 0.0042, 0.0038, 0.0046 /
DATA ENL03 / 940.0, 800.0, 680.0, 560.0, 460.0, 370.0, 280.0, 360.0,
1 440.0, 280.0, 80.0, 140.0, 250.0, 420.0, 710.0, 570.0, 470.0, 400.0,
2 360.0, 230.0, 320.0, 320.0, 330.0, 360.0, 400.0, 460.0, 520.0, 570.0,
3 590.0, 570.0, 490.0, 380.0 /
DATA NLC3 / 44.43, 43.46, 54.57, 71.130, 167, 76, 75, 97, 110, 133, 233,
1 157, 115, 129, 117, 103, 97, 102, 90, 86, 97, 97, 95, 97, 96, 96, 78, 51 /
COMMON /HCCCM/ HNOLAM, HHOSTR, HCOLSE, HRAC
COMMON /RCICOM/ ROTLAM, RCTEA, RCTLSE, ROTST
TCFAC = (273.15/T)**1.5
GC TO (100,200,300), N
CONTINUE
RADFAC = 1.58065E-20*DEN*TCFAC
TAUFAC = 4.00415E-18*SQRT(RM/T)*TCFAC*DEN
DO 110 I = 1, 250
1AU = TAUFAC*RCTST(I)*EXP(-1.43879*RCTLSE(I)/T)
1 * (1.0 - EXP(-14387.9/(ROTLAM(I)*T)))
1 HAC(I) = RA0FAC*ROTEA(I)*SFUN(TAU)
1 * EXP(-1.43879*(1.0E4/ROTLAM(I) + ROTLSE(I))/T)
110 CONTINUE
RETURN
200 CONTINUE
TAUFAC = 4.00415E-18*SQRT(RM/T)*CEN
TEFAC = (T - 273.15)/(T*273.15)*1.43879
SUM = 0.0
ON 210 I = 1, 434
HSTR = TCFAC*HOSTR(I)*EXP(TEFAC*RCTLSE(I))
TAU = TAUFAC*HNOLAM(I)*HSTR
HRAC(I) = TAU*SFUN(TAU)*EXP(-14387.9/(HCLAM(I)*T))

```

```

1 /H=CLAN(I)**4
  SLM = SUM + HRAD(I)
210  CONTINUE
  RADFAC = RAD/SUM
  DC 220 I = 1, 434
  HFACT(I) = HRAD(I)*RADFAC
220  CONTINUE
  RETURN
300  CONTINUE
  TGFAC = (238.0/T)**1.5
  TAUFAC = 4.8815E-18*SCRT(RP/T)*CEN*TGFAC
  TEFAC = (1 - 238.0)/(T*238.0)*1.43879
  HAVE = 997.5
  SLM = 0.0
  EC 310 I = 1, 14
  RLAM = 1.0E+4/HAVE
  TAU = TAU*FC*STRO3(I)*EXP(TEFAC*ENL03(I))*RLAM
  HFACT(I) = TAU*SFUN(TAU)*HLC3(I)*EXP(-1.43879*HAVE/T)
1 *(HAVE/1.0E4)**4
  HFACT(I + 300) = RLAM
  SLM = SUM + HFACT(I)
  HAVE = HAVE + 5.0
310  CONTINUE
  TGFAC = (281.0/T)**1.5
  TAUFAC = 4.8815E-18*SCRT(RP/T)*CEN*TGFAC
  TEFAC = (1 - 281.0)/(T*281.0)*1.43679
  DC 320 I = 15, 32
  RLAM = 1.0E+4/HAVE
  TAU = TAU*FC*STRO3(I)*EXP(TEFAC*ENL03(I))*RLAM
  HFACT(I) = TAU*SFUN(TP)*AL03(I)*EXP(-1.43879*HAVE/T)
1 *(HAVE/1.0E4)**4
  HRAD(I + 300) = RLAM
  SLM = SLM + HRAD(I)
  HAVE = HAVE + 5.0
320  CONTINUE
  RADFAC = RAD/SUM

```

DO 330 I = 1, 32
HRA0(I) = HRA0(I)*RA0FAC
330 CCNTINUE
RETURN
END

PSIR 730
PSIR 740
PSIR 750
PSIR 760
PSIR 770

```

SUBROUTINE RCTATE
DIMENSION WLT(250), EA(250)
DIMENSION ENL(250), ENL(250), ENERGY(250)
DIMENSION FCLAM(450), HHCSIR(450), HHOLSE(450), HRAU(600)
DIMENSION FOTLAM(250), RCTEA(250), RCTSE(250), RCTST(250)
COMMON /HCCCM/ HHOLAM, HHOSTR, HHOLSE, HRAU
COMMON /RCTCCM/ RCTLAM, RCTEA, RCTSE, RCTST
TEFAC = (273.15 - 287.0) / (273.15 * 287.0) * 1.43875
TCFAC = (287.0 / 273.15) * 1.5
      WRITE (2,16)
DO 110 I = 1, 434
      READ (1,21) HHCLAM(I), HHCSIR(I), HHCLSE(I)
      WRITE (2,21) HHCLAM(I), HHCSIR(I), HHCLSE(I)
      HHOLAM(I) = 1.0E+4 / HHOLAM(I)
      HHOSTR(I) = HHCSIR(I) * 8.0E3E-4 * TCFAC
      1 * EXP(TEFAC * HHCLSE(I))
      1 CONTINUE
      READ IN MOLECULAR CONSTANTS.
      READ (1,12) KMCLWT, RA, RE, SF, CIRCLE, CRFAC
      EAFAC = 64.0 * 3.1415927 * 4 * DIPOLE * DIPOLE / (3.0E-6 * 6256E-27)
      OR = CRFAC * SQR((273.15 / 1.43875) * 3 * 3.14159 / (RA * RE * RC))
      READ IN DATA FOR LINES
      REAC (1,6) ALINES
DO 130 I = 1, NLYNES
      READ (1,10) JU, KAU, KCU, JL, KAL, KCL, STR,
      1 ENL(I), ENL(I), ENERGY(I), SWI
      1 WRITE (2,10) JL, KAU, KCU, JL, KAL, KCL, STR,
      1 ENL(I), ENL(I), ENERGY(I), SWI
      1 WLT(I) = 10000.0 / ENERGY(I)
      EA(I) = EAFC * STR * ENERGY(I) * 3 / (JU * (JU + 1))
      EAFC(I) = EA(I) * SWT * JU * (JU + 1) / WLT(I)
      EAFC(I) = EAFC(I) * WLT(I) ** 4
      IF (ABS(ENL(I) - ENL(I) - ENERGY(I)) .GT. 6.005) WRITE (2,4)
      RCTST(I) = EAFC(I) / OR
      RCTEA(I) = EAFC(I) / OR
      FCTR 10
      FCTR 20
      FCTR 30
      FCTR 40
      FCTR 50
      FCTR 60
      FCTR 70
      FCTR 80
      FCTR 90
      FCTR 100
      FCTR 110
      FCTR 120
      FCTR 130
      FCTR 140
      FCTR 150
      FCTR 160
      FCTR 170
      FCTR 180
      FCTR 190
      FCTR 200
      FCTR 210
      FCTR 220
      FCTR 230
      FCTR 240
      FCTR 250
      FCTR 260
      FCTR 270
      FCTR 280
      FCTR 290
      FCTR 300
      FCTR 310
      FCTR 320
      FCTR 330
      FCTR 340
      FCTR 350
      FCTR 360

```

```

FC1R 370
FC1R 380
FC1R 390
FC1R 400
FC1R 410
FC1R 420
FC1R 430
FC1R 440
FC1R 450
FC1R 460
FC1R 470
FC1R 480
FC1R 490
FC1R 500
FC1R 510

FCILAP(1) = WYLTH(1)
FCILSE(1) = ENL(1)
CONTINUE
RETURN
4 FORMAT (24H ERROR IN ABOVE CARD)
6 FORMAT (6I16)
8 FORMAT (6E12.4)
10 FORMAT (6I3,F12.6,3F9.2,F5.1,E12.3,F12.3)
12 FORMAT (4F12.4,E12.4,F12.6)
14 FORMAT (1X)
16 FORMAT (1I12)
21 FORMAT (F6.2,F10.4,F8.2)
22 FORMAT (F10.5,E12.4,F11.2)
23 FORMAT (F10.5,E12.4,F11.2,E12.4)
END
130

```

```

FUNCTION SIMP (A,H,K)
DIMENSION A(3)
IF (K == 2) 100,110,120
100  CONTINUE
      SIMP = (8.0*A(2) + 5.0*A(1) - A(3))*H/12.0
      RETURN
110  CONTINUE
      SIMP = (8.0*A(2) + 5.0*A(3) - A(1))*H/12.0
      RETURN
120  CONTINUE
      SIMP = (4.0*A(2) + A(1) + A(3))*H/12.0
      RETURN
END

```

```

FUNCTION SFUN (TAU)
T = ABS(TAU)
IF (T .GT. 4.0) GO TO 110
X = (T - 2.0)*0.5
SFUN = (((0.001061*x - 0.004288)*x + 0.013686)*x - 0.042491)
1 *X + 0.14632)*X - 0.267057)*X + 0.556485
RETURN
110  CONTINUE
IF (T .GT. 4.0) GO TO 120
X = (T - 7.0)/3.0
SFUN = (((((0.000347*x - 0.001167)*x + 0.03148)*x - 0.004545)
1 *X + 0.028248)*X - 0.081972)*X + 0.247900
RETURN
120  CONTINUE
Y = ALOC(1)
X = 1.0/Y
SFUN = (((((0.067876*x - 0.268698)*x + 0.264568)*x
1 - 0.265167)*x + 0.325368)*x + 1.128375)*SCR1(Y)/T
RETURN
END

```

```

FUNCTION CINT (A,H1,H2,K)
DIMENSION A(3)
HS = H1 + H2
IF (K - 2) 130,117,127
100  CONTINUE
  CINT = ((A(2)*HS - A(1)*H2 - A(3)*H1)*H2**HS)
  1 + (A(1) + A(2))*0.5)*H1
  RETURN
110  CONTINUE
  CINT = ((A(2)*HS - A(1)*H2 - A(3)*H1)*H2 / (6.0*H2**HS)
  1 + (A(2) + A(3))*0.5)*H2
  RETURN
120  CONTINUE
  QINT = (A(2)*HS - A(1)*H2 - A(3)*H1)*(H1**3 + H2**3)
  1 / (6.0*HS*H1*H2) + (A(1)*H1 + A(2)*HS + A(3)*H2)*0.5
  RETURN
END

```

```

SUBROUTINE FILTER (SPEC,RAD,VLTR,^)
DIMENSION SPEC(201),RAD(450),VLTR(450)
DO 150 N = 1, N
  RT = VLTR(I)
  RADT = RAD(I)
  JS = (RT - 5.25)*10.0 + 2.0
  JF = (RT - 4.75)*10.0 + 1.0
  IF (JS .LT. 1) JS = 1
  IF (JF .GT. 201) JF = 201
  IF (JS .GT. JF) GO TO 150
  DO 120 J = JS,JF
    RLAM = (J - 1)*0.1 + 5.0
    SPEC(J) = SPEC(J) + (0.25 - ABS(RLAM - RT))*RAUT*16.0
  120 CONTINUE
  150 CONTINUE
  RETURN
END

```

```

      FLTR 10
      FLTR 20
      FLTR 30
      FLTR 40
      FLTR 50
      FLTR 60
      FLTR 70
      FLTR 80
      FLTR 90
      FLTR 100
      FLTR 110
      FLTR 120
      FLTR 130
      FLTR 140
      FLTR 150
      FLTR 160
      FLTR 170

```

```

SUBROUTINE RCTISTR (RAC, RM, EVFF, T, CEN, STR, FS, CS, RS, AF, NC, F, G, R)
DIMENSION P(1:10), Q(1:10), R(1:10), PS(1:10), QS(1:10), RS(1:10)
NC • EC. 1 FOR ALL LINES
ND • EG. 2 FOR ALTERNATE LINES
NP • EG. 1 FOR PARALLEL EANC
NP • EG. 2 FOR FERPENICCLPF EANC
SIG = 1.43879*EVPP/T
PS(1) = 0.0
QS(1) = 0.0
RS(1) = 1.0
SUM = 1.0
AJ = ND
DJ = ND
IF (AF • G1. 1) GO TO 200
DO 110 I = 2, 100
FAC = EXP (-SIG*AJ* (AJ + 1.0))
PS(I) = AJ*FAC
QS(I) = 0.0
FS(I) = (AJ + 1.0)*FAC
SUM = SUM + PS(I) + RS(I)
AJ = AJ + DJ
110 CCNTINUE
GO TO 300
200 CCNTINUE
DO 210 I = 2, 100
FAC = 0.5*EXP (-SIG*AJ* (AJ + 1.0))
PS(I) = (AJ - 1.0)*FAC
RS(I) = (AJ + 2.0)*FAC
QS(I) = PS(I) + RS(I)
SUM = SUM + 2.0*QS(I)
AJ = AJ + DJ
210 CCNTINUE
300 CCNTINUE
TAUFAC = 4.8815E-18*SCRT (RM/T)*CEN*STR/SUM
SUM = 0.0
DO 310 I = 1, 100

```

```

PTAL = FS(I)*P(I)*TAUFAC
CTAL = GS(I)*G(I)*TAUFAC
RTAU = RS(I)*R(I)*TAUFAC
PS(I) = PTAL*SFUN(PTAU)*EXP((-14387.9/(P(I)*T))/P(I))**4
GS(I) = Q1AU*SFUN(QTAU)*EXP((-14387.9/(G(I)*T))/G(I))**4
RS(I) = R1AL*SFUN(RTAU)*EXP((-14387.9/(R(I)*T))/R(I))**4
SLM = SUM + PS(I) + QS(I) + RS(I)
CONTINUE
RAOFAAC = RAO/SUM
DO 320 I = 1, 100
PS(I) = PS(I)*RAOFAAC
GS(I) = QS(I)*RAOFAAC
RS(I) = RS(I)*RAOFAAC
CONTINUE
RETURN
END
310
320

```

```

FSIR 370
FSIR 380
FSIR 390
FSIR 400
FSIR 410
FSIR 420
FSIR 430
FSIR 440
FSIR 450
FSIR 460
FSIR 470
FSIR 480
FSIR 490
FSIR 500
FSIR 510
FSIR 520

```

1 TA0FF=OUTPUT, TA0FF2, TA0FF3=TINPUT,
2 VEFCTN 2
3 COMMUN AYLM, SERTD, X, Y

4 DIMENSION AYLM(201), SERTD(201,12)
5 DIMENSION X(201), Y(2412)
6 DIMENSION XRD(17), YRD(17)
7 DIMENSION JREAM(12)
8 DIMENSION TENT(6)
9 DATA TENT(2), TENT(3) /10H, 0FCGF5, 10H 7023, 0-4/
10 DATA JREAM /16, 15, 14, 12, 16, 15, 14, 12, 16, 15, 14, 12/
11 DATA TENT /10H /5X, 5HST, 10HPT, 6X, 3HFN, 10H, 7X, 5HTOT,
12 10HAL, 6X, 5HT, 10HMF /1X, 3F1, 5H0.2/ /
13 6 FORMAT (1X, T5)
14 6 FORMAT (1X, F6.2, X, F9.2)
15 6 FORMAT (1H1)
16 CALL SFRND (SFRND)
17 CALL DATE (TENT(1))
18 NH = 6
19 WRITE (6, 16)
20 SX = 9.0
21 SY = 14.0
22 NH = 2
23 CALL CRTPL (TENT1, 1.0, 17.0)
24 CALL PL01 (1.0, 1.0, -2)
25 QFAN (5, 5) NCASES
26 MPTTF (6, 6) NVAL, YMCN
27 QFAN (5, 5) NVAL, YMCN
28 MPTTF (6, 6) NVAL, YMCN
29 QFAN (5, 5) NCASES
30 MPTTF (6, 6) NVAL, YMCN
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33 QFAN (5, 5) NCASES
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232 MPTTF (6, 6) NVAL, YMCN
233 QFAN (5, 5) NCASES
234 MPTTF (6, 6) NVAL, YMCN
235 QFAN (5, 5) NCASES
236 MPTTF (6, 6) NVAL, YMCN

```

WRTTF (5,10) WUMTN, WUMDX
TNS = 10.0*WUMTN - 49.0
TF (TNS - 1, 1) TNS = 1
TNF = 10.0*WUMDX - 48.0
TF (TNF, GT, 201) TNF = 201
NX = TNF - TNS + 1
NY = 12*NX
NC 300 NR = 1, ?
SCAN (2) AVLAM
NC 110 T = 1, NX
X(T) = AVLAM(TNS + T - 1)

110 CONTINUE
CALL LTNSCA (X,NX,SX,YMTN,DX,KNY)
CAD = SX/FLNAT(KNY/10)
SX = CAD*DX
NCAD = MIN(KNY,10)
NC 250 NSPC = 1,
QFAN (2) SNTFQ1
T9 = 1
NC 130 J = 1, 1
NC 120 T = 1, NX
Y(TJ) = CORTOA(TNS + T - 1, J)
TJ = TJ + 1
NC 110 T9 = 1

120 CONTINUE
CALL LONGRA (Y,NY,SY,MTNY,MAXY,3)
CALL STREAM (15)
CALL LTNAXS (SY,0,0,YRL,-NXL,DX,
1 90.0, XMTN, CX, CAD, NH, NCAD)
CALL LTNAYC (0,0,0,0,YRC, NXL, CX,
1 90.0, XMTN, CX, CAD, NH, -NCAD)
CALL LOGAXC (SY,0,0,YRL,NYL,SY,
1 180.0, MTNY, MAXY, 1)
CALL LOGAXS (SY,SY,YRL,-NYL,SY,
1 NC 110.0, MTNY, MAXY, 1
MOLG CDTN (FXT(X(CY/NCAD - 0.0), CAD, SY)

```

CALL CRDN (MTNY + 1 - MAXY, SY/ELDAT(MAXY - MTNY, SX))
DO 160 T = 1, NY
Y(T) = SY - V(T)
150 CONTINUE
DO 200 J = 1, 12
CALL SFRAW (J, FAM(J))
ZJ = JU - 1 + NX + 1
CALL NULINE (Y(TJ), X, NX, SY, SX)
200 CONTINUE (1.5, 1.5)
250 CONTINUE
300 CONTINUE
REWIND 2
400 CONTINUE
DATA -SFRAW 1
CALL SECOND (SFRAW)
SFRAW = RECFD - SFRAW
WRITE (1W, TENT) SFCA, SFCA, SFCA, SFCA
STOP
FND
906

TCRT 730
TCRT 740
TCRT 750
TCRT 760
TCRT 770
TCRT 780
TCRT 790
TCRT 800
TCRT 810
TCRT 820
TCRT 830
TCRT 840
TCRT 850
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TCRT 870
TCRT 880
TCRT 890
TCRT 900
TCRT 910
TCRT 920

SaudiaOrientis - Thesaurus - X. N. S. A. M. T. U. Y. K. M. I.

THE SCALING ALGORITHM IS BASED ON THE PERTURBATION THAT THE PLANT WILL USE AT THE LEAST SEVENTY PER CENT OF THE LENGTH OF A THREE AXES.

```

DIMENSTON A(14),KA(14),KR(14),X(100)
DATA A /1.0,1.2,1.5,1.0,2.0,2.0,2.4,3.0,4.0,5.0,6.0,7.0,5,
      9.0,10.0,12.0/
DATA KA /10,12,15,9,20,12,15,10,10,12,15,9,10,12/
DATA KR /44,37,74,32,44,33,34,44,44,33,34,32,44,33/
X4X = X(1)

```

```

XMN = XMX
ADX = 0.0
DO 110 I = 2, N
  XMX = AMAX1(XMX, X(T))
  ...
  XMN = AMIN1(XMN, X(T))
110

```

110 CONTINUE
 $SX = XMX - XWN$
 $K = 0$

120 CONTINUE

60 71 1 20
X = X - 1
S X = S X * 0.9999999999999999
S E (S X * G F . 0 . 9999999999999999)

1130--CANTYNUE TF (SX .LT. 10.0) GN TO 140

```

X = 0.175
K = K + 1
SN TO 170
140 CONTNUF
-170-150 T = 1.0 14
TF (SY ST 1.0005*A(T)) GO TO 150

```

```

ST = A(T)*IN.0***K
DX = ST/ELDAT(KA(T))
XMTN = XMN - AMON(XMN,DX),DX
DX = ST/S

```

LNSC 10	LNSC 20	LNSC 30	LNSC 40	LNSC 50	LNSC 60	LNSC 70	LNSC 80	LNSC 90	LNSC 100	LNSC 110	LNSC 120	LNSC 130	LNSC 140	LNSC 150	LNSC 160	LNSC 170	LNSC 180	LNSC 190	LNSC 200	LNSC 210	LNSC 220	LNSC 230	LNSC 240	LNSC 250	LNSC 260	LNSC 270	LNSC 280	LNSC 290	LNSC 300	LNSC 310	LNSC 320	LNSC 330	LNSC 340	LNSC 350	LNSC 360
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KON = K0 (T)
IF ((XMX - XMIN)/DX .LT. S*1.00005, GO TO 150
150 CONTINUE
160 CONTINUE
170 NO 220 T = 1, N
X(T) = (X(T) - XMIN)/DX
180 CONTINUE
190 RETURN
200 CONTINUE
210 RETURN
220 CONTINUE
230 RETURN
240 RETURN
250 RETURN
260 RETURN
270 RETURN
280 RETURN
290 RETURN
300 RETURN
310 RETURN
320 RETURN
330 RETURN
340 RETURN
350 RETURN
360 RETURN
370 RETURN
380 RETURN
390 RETURN
400 RETURN
410 RETURN
420 RETURN
430 RETURN
440 RETURN
450 RETURN
460 RETURN

SUPPORTN LOCSCA (X,N,S,MIN,MAX,K)
IF K IS POSITIVE, K LOC CYCLES WILL BE PRODUCED.
IF K IS NEGATIVE, INPUT VALUE OF MTN WILL BE USED.

```
      C      DTMFNSION X(100)
      MTNSAV = MTN
      XX = ALONG10(ABRS(X(1)) + 1.0E-99)
      X(1) = XX
      XMAX = XX
      XMIN = XX
      DO 110 I = 2, N
      XX = ALONG10(ABRS(X(I)) + 1.0E-99)
      X(I) = XX
      XMAX = AMAX1(XMIN,XX)
      XMIN = AMIN1(XMIN,XX)
      110  CONTINUE
      MAX = XMAX
      MTN = XMIN
      TF (FLOAT(MTN) .LT. XMAX) MTN = MAX + 1
      TF (FLOAT(MTN) .LT. XMIN) MTN = MTN - 1
      TF (K .LT. 0) MTN = MTNSAV
      IF (K .LE. 0) GO TO 120
      MTN = MAX0(MIN,MAX - K)
      120  CONTINUE
      FAC = SFLOAT(MAX - MIN)
      XMTN = MTN
      DO 130 I = 1, N
      X(I) = (X(I) - XMIN)*FAC
      IF (X(I) .LT. 0.0) X(I) = 0.0
      130  CONTINUE
      RETURN
      END
```



```

160  ANDX = -ARV
      CONTINUF
      XA = XA - 10.1*SN - 0.025)*SANDJ - 0.0954*RANJ
      YA = YA + 10.1*SN - 0.025)*RANDJ - 0.0954*RANDJ
170  CONTINUF
      N = N + 1
      SFAC = 0.0429*SANDJ
      SFAC = 0.0620*SANDJ
      DO 200 T = 1, N
      IF (NH * LT. 0) GO TO 180
      CALL NMWDFD (XA, YA, HFTCHT, ARCV, THFTA, 3)
      ARSV = ARSV - DTX
      GO TO 190
      CONTINUF
      TAD = 1
      IF (ARSV(ARSV) .GE. 10.0)
      1 IFTX(ARSV10(ARSV)) + 1.0F-6) + 1
      YA = XA - SFAC*FLONT(TAD - 1)
      YA = YA - SFAC*FLNAT(TAD - 1)
      CALL NMWDFD (XA, YA, HFTCHT, ARCV, THFTA, 3)
      ARSV = ARSV - DTX
      CONTINUF
      XA = XA - GAP*CTH
      YA = YA - GAP*STH
      190 CONTINUF
      IF (NH .GE. 0) GO TO 210
      ANC = MC
      XA = X + (S2 - 0.07*ANR*SANDJ)*CTH - (0.18*SN - 0.035)*SANDJ
      YA = Y + (S2 - 0.07*ANR*SANDJ)*STH + (0.18*SN - 0.035)*SANDJ
      HFTCHT = 0.07*DNU
      CALL SYM001 (XA, YA, HFTCHT, RCD, THETA, MC)
      RETURN
210  CONTINUF
      TNC = MC + 7
      XA = X + (S2 - 0.07*TNC*SANDJ)*CTH - (0.18*SN - 0.0375)*SANDJ
      YA = Y + (S2 - 0.07*TNC*SANDJ)*STH + (0.18*SN - 0.0375)*SANDJ
      LMAX1060
      LMAX1070
      LMAX1080

```

```

HFTIGHT = 0.17*ANJ
CALL SYMPNL (XA,YA,HFTIGHT,PCD,THETA,MC)
TC (F*E0. 0.0) RETURN
XA = YA + ((TNC - 5.0)*0.06*ANJ)*FTH
YA = YA + ((TNP - 6.0)*0.06*ANJ)*STH
CALL SYMPNL (XA,YA,HFTIGHT,W,THETA,5)
IF (F - 1.0) 220,250,270
220 CONTINUE
XA = YA + 0.30*CANJ - 0.035*SANJ
YA = YA + 0.30*SANJ + 0.035*CANJ
GO TO 240
230 CONTINUE
XA = YA + 0.30*CANJ - 0.035*SANJ
YA = YA + 0.30*CANJ + 0.035*SANJ
240 CONTINUE
HFTIGHT = 0.05*ANJ
CALL NUMBER (XA,YA,HFTIGHT,F,THFTA,-1)
250 CONTINUE
RETURN
END

```

```

SUBROUTINE LGAXS (X, Y, PRM, NCF, C, TURTA, MIN, MAX, NTEST)
DTMENSTN N PDC(9)
SN = 1.0
TF (NCF * LT. 0) SN = -1.0
FAC = 1.0
TH = 0.017453294*TURTA
CTH = CTH(TH)
STH = STH(TH)
CFAC = CTH*S/FLNAT(MAX - MIN)
SFAC = STH*S/FLNAT(MAX - MIN)
XL = 0.1*SN*CTH*FAC
YL = 0.1*SN*CTH*FAC
XM = 1.05*XL
YM = 1.05*YL
CALL PLOT (X + XM, Y - YM, 2)
XA = X
YA = Y
N = 0
CONTINUE
D = 2.0
Q = 1.0
XR = XA
YR = YA
150 CONTINUE
CALL PLOT (XB, YR, 2)
PDLNG = ALOC10 (P/Q)
XB = XB + CFAC*D*Q
YB = YB + SFAC*D*Q
CALL PLOT (XB, YB, 2)
TF (P .F. 0. 10, 0) GO TO 160
P = P + 1.0
Q = Q + 1.0
CALL PLOT (XA + XL, YR - YM, 2)
GO TO 150
160 CONTINUE
CALL PLOT (XA + YM, YB - YM, 2)

```

```

N = N + 1
XA = XA + CFAC
YA = YA + SFAC
TF (N = MAX + MIN . LT. 0) GO TO 300
IF (TEST . EQ. 0) GO TO 300
FAC = 0.7*FAC
XP = MTN
XA = X
YA = Y
170 CONTINUE
XA = XA - ((0.325*SN - 0.1)*STH + 0.235675*CTH)*FAC
YA = YA + ((0.325*SN - 0.1)*CTH - 0.235675*STH)*FAC
CASE = 10.0
IF (XP . NE. 0.0) GO TO 180
XA = XA + 0.064475*CTH*FAC
YA = YA + 0.064175*STH*FAC
CASE = -1.0
180 CONTINUE
CTH = NUM980 - TXB, YB, 0.18*FAC, RASE, THETA, -1)
TF (XP . LT. 0.0) GO TO 200
FF EXP . SFAC. 0.0) .. GO TO -236
TF (XP . EQ. 1.0) GO TO 230
FF EXP . CT. 10.0) GO TO 190
190 CONTINUE
XT = XA - (0.3143*CTH - 0.1*STH)*FAC
YT = YB + (0.3143*STH + 0.1*CTH)*FAC
60 TO 220
200 CONTINUE
210 CONTINUE
IF (XP . GT. -10.0) GO TO 210
XT = XA + 10.3713*CTH - 0.125*STH)*FAC
YT = YB + 10.3713*STH + 0.125*CTH)*FAC
220 CONTINUE
CALL NUM960 (XT, YT, n, 1*FAC, XD, THETA, -1)
230 CONTINUE
XA = XA + SFAC

```

```

YA = YA + S*AC
XP = XP + 1.0
TF (XP - 1.0 - FLOAT(MAX) .LT. 0.0)  GO TO 170
NC = FLOAT(NJ)*SN
T = S/EN
XA = X + (T - NJ*0.37155 - 0.05725)*0.5*CTH -
1 (0.6*SN - 0.1)*STH)*FAC
YA = Y + (T - NJ*0.17155 - 0.05725)*0.5*STH +
1 (0.6*SN - 0.1)*CTH)*FAC
NJ = NJ
CALL SMMN (XP, YD, 0.2*FAC, RDN, THETA, ND)
300 CONTINUE
RETURN
END

```

```

SUBROUTINE: SPTD (NL,SPACE,S)
CALL STREAM (12)
NL = TARE(NL)
AX = 0.0
AY = 0.0
TF (SPACE, 0.0) GO TO 200
TF (NL, 0) GO TO 209
TF (NL,GT, 0) GO TO 120
BX = 0.0
BY = S
DX = AYS (SPACE)
DY = 0.0
GO TO 130
120 CONTNUF
BX = S
BY = 0.0
DX = 0.0
DY = AYS (SPACE)
130 - CONTINUE
IT = 0
DO 150 IT = 1, NT
AX = AX + DX
AY = AY + DY
AX = AX + DX
BY = BY + DY
IT = 1 - IT
TF (IT,LT, 0) GO TO 200
TF (IT,GT, 0) GO TO 140
CALL PLOT (AX, AY, 7)
CALL PLOT (AX, AY, 2)
GO TO 150
140 CONTNUF
CALL PLOT (AX, AY, 7)
CALL PLOT (AX, AY, 2)
CONTNUF
150 CONTNUF
200 CONTNUF
CALL STREAM (14)
RFTUPN
END

```

```

SURRENTNF NULTF (X,Y,N,SX,SY)
DTMFNSTON X(100),Y(100)
NL = 0.1
SX = SX + NL
XA = X(1)
YA = Y(1)
TPNA = 2
IF (XA .LT. -NL) TONA = 2
TF (XA .GT. SX) TONA = 2
TF (YA .LT. -NL) TPNA = 3
TF (YA .GT. SY) TPNA = 2
CALL PLOT (XA,YA,TA,TPNA)
DO 150 T = TPNA, N
TPNA = T
XA = X(T)
YA = Y(T)
TPNA = 2
IF (XA .LT. -NL) TONA = 2
TF (YA .LT. -NL) TPNA = 2
TF (YA .GT. SY) TPNA = 2
TPN = 2
IF (TPNA + TONA .NE. 4) TON = 2
CALL PLOT (XA,YA,TA,TPN)
CONTNUF
RTURN
END
150

```